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Project A. Technical guidance for identifying an appropriate emission scenario

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Project A. Technical guidance for identifying an appropriate emission scenario

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On behalf of the Federal Environmental Agency

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16. Kurzfassung

Der vorliegende technische Leitfaden wurde für Stoffhersteller, Importeure und nachgeschaltete Stoffanwender entwickelt. Er ermöglicht es diesen, ein fachlich begründetes Emissionsszenario mit adequaten Emissionsfaktoren und Emissionsperioden zu identifizieren. Der Leitfaden umfasst die Emissionsschätzung ins Abwasser, in die Luft und in den Boden für relevante Lebenszyklen (z.B. Produktion und Formulierung), Funktionen, Anwendungen und Prozesse eines Stoffes in der Industrie und in der Gesellschaft.
Der entscheidende Teil des Leitfadens ist ein interaktiver Entscheidungsbaum, welcher zu einer bestimmten Zelle in einer sog. Matrix hinführt. Die Matrix wiederum beinhaltet alle Informationen hinsichtlich verfügbarer Emissionsschätzmodule. Die Informationen in der Matrix basieren auf Emissionsschätzmodulen, die aus bestehenden Emissionsszenario-Dokumenten abgeleitet wurden. Sind für bestimmte Situationen keine Emissionsszenario-Dokumente verfügbar, werden die Default-Werte des EU Technical Guidance Document on Risk Assessment (2003) verwendet. Die Navigation durch den Entscheidungsbaum erfolgt mittels sukzessiver Auswahl der richtigen Parameter (Identifikatoren) für jeden Lebenszyklus eines Stoffes. Die Hauptparameter (Hauptidentifikatoren), wie z.B. die relevante Industriekategorie und Verwendungskategorie, das chemische Produkt (Zubereitung) oder das halbfertige Produkt (performance package), werden jeweils dargestellt und definiert.
Die Methodologie des Entscheidungsbaumes wurde für zwei Beispielstoffe aus verschiedenen Industriezweigen (d.h. eine Photochemikalie und ein Kunststoffadditiv) erarbeitet und endete in der Auswahl eines fachlich begründeten Emissionsszenarios für diese Stoffe und deren Anwendungsbereich.

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16. Abstract

A tool has been developed for manufacturers, importers, and downstream users of chemical substances to facilitate the finding of the appropriate emission scenarios with the best estimates for emission factors and emission period(s). The tool comprises the making of emission estimates to wastewater, air, and soil for all relevant functions and life cycle stages, e.g. production and formulation, in all possible applications and processes throughout industry and society.
The crucial part of the tool is the interactive decision tree leading to the required location of a matrix, which contains all information on available emission estimates (modules). The matrix information is based on emission estimation modules derived from existing emission scenario documents and, if not available, default values from the EU Technical Guidance Documents. The routing through the decision tree is determined by selecting the right parameters (identifiers) for each life. cycle stage. The main identifiers, such as the relevant industrial category, use category, the type of chemical product and semi-finished preparation (performance package), are overviewed and defined.
The methodology has been tested and illustrated for two substances in different industrial categories, i.e. a photochemical and a plastic additive, rendering appropriate emission scenarios.

17. Keywords
Industrial chemical, emission estimation, exposure assessment, emission scenario, REACH

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List of abbreviations

CP	Chemical Products; used as label for Identifier 6
CSA	Chemical Safety Assessment
CSR	Chemical Safety Report
EEM	Emission Estimation Module
ES	Exposure Scenario
ESD	Emission Scenario Document
EUSES	European Union System for the Evaluation of Substances
HEDSET	EC/OECD Harmonised Electronic Data SET
HPVC	High Production Volume Chemical
IC	Industrial Category; also used as label for Identifier 2, 5, 7 and/or 9
ID	Identifier
LPVC	Low Production Volume Chemical
NACE	Nomenclature générale des Activités économiques dans les Communautés Européennes
NAICS	North American Industrial Classification System
PBT	Persistent, Bioaccumulative, and Toxic
PL	Production Level; used as label for Identifier 3
PR	Process; used as label for Identifier 10
REACH	Registration, Evaluation, and Authorisation of CHemicals
RMM	Risk Management Measure
SP	Semi-finished Preparation; used as label for Identifier 4
TGD	Technical Guidance Document
TU	Type of Use; used as label for Identifier 8
UC	Use Category; also used as label for Identifier 1
vPvB	very Persistent and very Bioaccumulative

1. Introduction

A new regulation concerning the Registration, Evaluation, and Authorisation of Chemicals (REACH) was proposed by the European Commission on October 29, 2003 (EC, 2003a). The regulation puts major responsibility on industry for ensuring the safe manufacture, import, and use of chemicals throughout the chemical supply chain and for documenting this in their registration dossiers. Manufacturers and importers are required to conduct a chemical safety assessment (CSA) for substances manufactured or imported in a quantity above 10 tonnes per year. The CSA shall comprise an assessment of the intrinsic hazards of the substance including development of the classification and labelling, derivation of no-effect-levels for human health and the environment, and PBT (Persistent, Bioaccumulative, and Toxic) and vPvB (very Persistent and very Bioaccumulative) assessment. For substances meeting the criteria for classification as dangerous or assessed to be a PBT or vPvB, an exposure and risk assessment is also required with the purpose of documenting the safe manufacture and use, including risk management measures (RMMs).
An important aspect of the exposure assessment is the estimation of emissions on the basis of the information provided in the so-called exposure scenario (ES). From the start of quantitative risk assessment of substances, the emission estimation appeared to be one of the most problematic areas because of the huge diversity in applications and functions. Furthermore, emission estimates are often worst case and validation studies on the risk assessment of substances in the EU have shown that the uncertainty in the environmental risk assessment is mostly dominated by uncertainty in emission estimation (Jager et al., 1998; EC, 2004). Hence, the development of a facilitating tool in making adequate emission estimates is highly mandatory.

1.1 Exposure scenarios

An exposure scenario is a description of a control strategy for substances, giving realistic conditions for use for manufacture or identified use(s) of a substance, a group of substances or a preparation. It prescribes necessary Risk Management Measures (RMMs) that shall be in place during manufacture or use of a substance, including service life and waste phase, under a given set of operational conditions. The exposure

scenario is meant for risk management at the various life cycle stages (Figure 1) to ensure safe handling and adequate control of risk related to human health (workers and consumers) and the environment. The exposure scenario may be refined in an iterative process until adequate control of risks has been demonstrated.

A "tentative" ES is a set of assumptions on how a process is conducted and which risk management measures that are or should be implemented. The tentative ES forms the starting point for the exposure assessment and risk characterisation, which shall be conducted as part of the CSA. During the iterative CSA, the ES (as well as the hazard information) may be revised until it is shown that risks are adequately controlled during conduction of the process covered by the ES. A "tentative ES can be developed from typical operational conditions for a process (e.g. industrial process or consumer use) and typical implemented RMMs as a starting point. It should be clear which RMMs are included as well as their mitigating effects.

The "final" ES is the outcome of the CSA and is part of the chemical safety report (CSR), which should document that risks are adequately controlled. The CSR shall be submitted to authorities as part of the registration dossier. The ES includes information on operational conditions and RMMs for the process that may be subject to control and enforcement by authorities. If adequate control of risks during manufacture and use can be demonstrated with the tentative ES, the tentative ES will then become the final ES for the substance(s) and process(es) considered.

1.2 Emission estimation

For emission estimation the EU Technical Guidance Document on Risk Assessment (TGD; EC, 2003b) contain chapter 7 with Emission Scenario Documents (ESDs), which describe and quantify emissions for specific industrial processes and uses (EC, 2003b; OECD, 2005). In case ESDs are not available the more generic default emission estimation values contained in "A- and B-tables" of the TGD (EC, 2003b) are used. Several of these ESDs as well as the tables with defaults have been implemented in risk assessment software: the European Union System for the Evaluation of Substances (EUSES; EC, 2004). In practice, however, the selection of emission factors for manufacture and use of chemicals is problematic in view of the large variety of processes and uses of chemicals.

It is precisely the aim of this project to give guidance to manufacturers, importers, and downstream users on how to find the appropriate emission scenario with the best estimates for emission factors and emission period(s). This guidance should help them to correctly estimate emissions to air, soil, wastewater, and, if possible, solid waste.

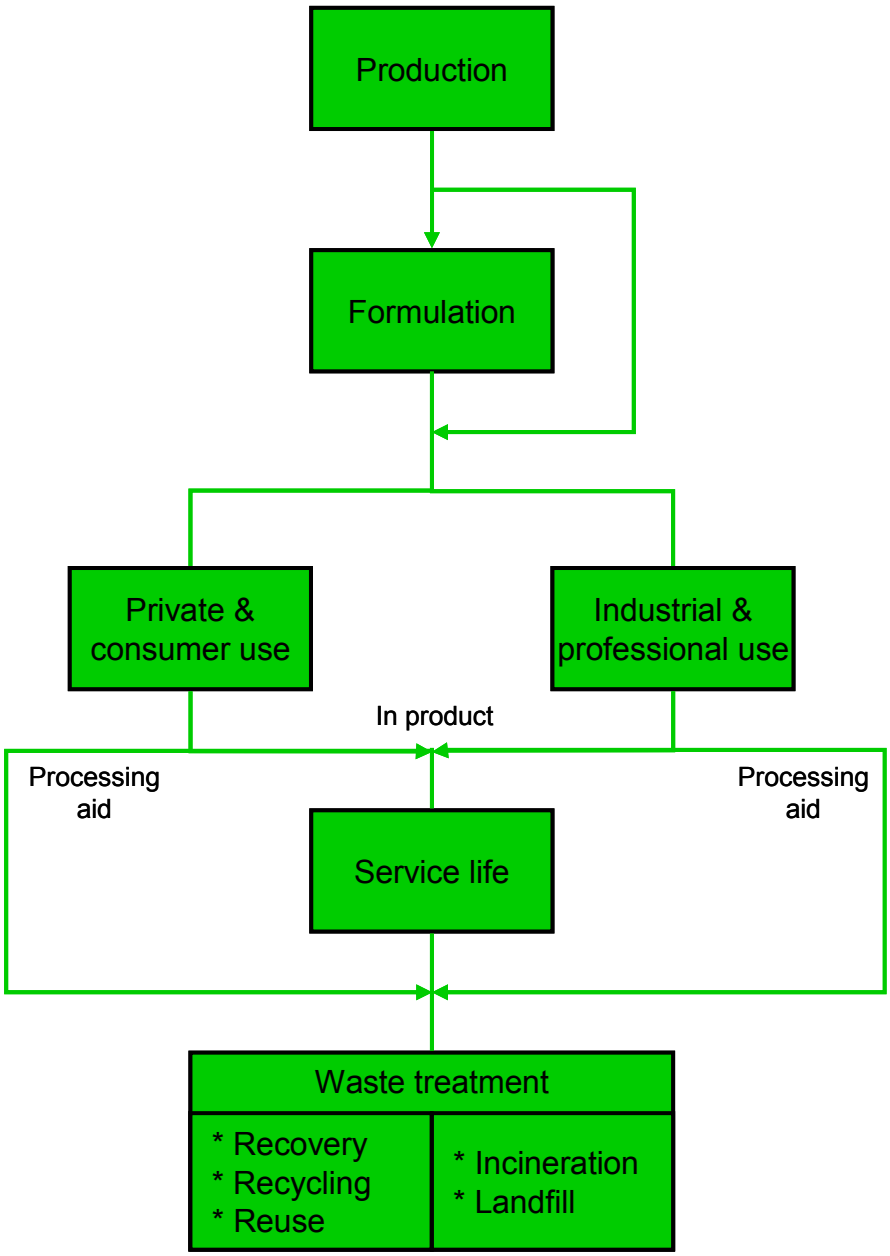

Figure 1 Schematic representation of the general form of the life cycle of a substance

1.3 The OECD matrix project

The project has as full title 'Branch and product related emission estimation tool for manufacturers, importers, and downstream users within the REACH system'. The title that is usually referred to is 'The OECD matrix project'. The project has been split in two parts, Project A and Project B. The total project aims at the development of a matrix filled with emission scenarios that should be available in order to enable the emission estimation for all relevant life cycle stages and functions in all possible applications and processes throughout industry and society. A short name for the project therefore is “Matrix Project”. Project A, the subject of this report, aims at the development of a guiding tool for choosing the appropriate emission scenario in the matrix based on information contained in the exposure scenario as defined above. This information comprises data such as industrial category (IC) for the use area of the substance, use category (UC) for the purpose of the substance, way of application of the substance or a chemical product containing the substance etc. Such data items are called identifiers (IDs). For emission scenarios to be used for emission estimation the required identifiers may vary according to the specific use and application of the substance/chemical product. The objective of this report is the description of how the identifiers are brought together in a kind of target funnel (Figure 2), which yields the emission scenarios. As the identifiers vary a certain path has to be followed to ensure that the identifiers needed are selected and evaluated one by one.

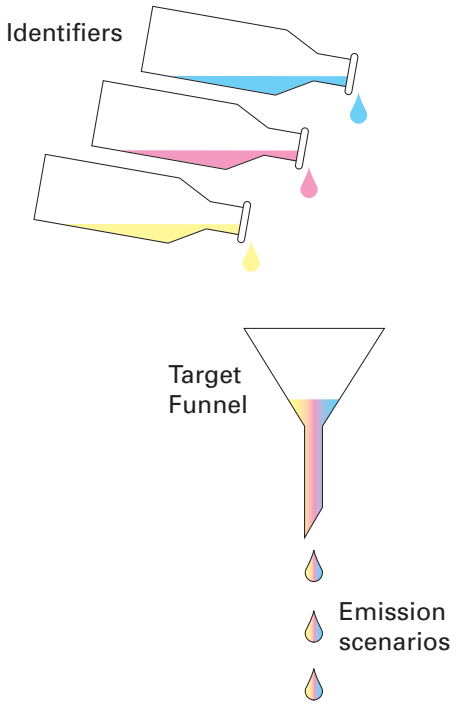

Figure 2

Selection of emission scenarios for relevant stages of the life cycle with the aid of identifiers, depicted as a kind of target funnel.

The evaluation of one identifier leads to the selection of the next identifier. This is done by means of a decision tree which is described in Chapter 3. If there is no specific emission scenario (or ESD) the correct A- and B-tables of the TGD should be identified (see Annex 1).
Project B will lead to the development of the matrix and guidance, including manuals and software, for the emission estimation itself. The guidance will only be available for two exemplified industrial branches.

2. Methods

Exposure assessment under REACH entails two steps: (1) development of exposure scenarios and (2) Exposure estimation (EC, 2003a). The first element of exposure estimation is the emission estimation. In order to assure that the correct emission modules will be used several data items (parameters) are necessary. These data items have been named "identifiers". Identifiers may be different depending on the stage of the life cycle (see Figure 1), the type of application, the process, the industrial branch etc. The number of identifiers needed is variable as well. This is illustrated in Figure 2, where the target funnel is depicted as the instrument that yields the emission scenarios to be applied for the relevant stages of the life cycle of the chemical.

2.1 Data requirements and availability

The data to be supplied by the registrant of a substance in an ES under REACH have not been defined yet. It is most likely that they will at least consist of the same basic data the notifier of a new substance at present has to provide. These data comprise the following:

1 physico-chemical properties,
2 industrial category,
3 use category,
4 detailed information on envisaged use.

Sub 1

The physicochemical properties consist of vapour pressure, melting point, boiling point, water solubility, and octanol-water partition coefficient. These parameters are usually not used and needed as identifiers.

Sub 2

For the industrial category the notifier specifies the category where the substance is used or applied in a preparation such as a chemical product like paint. In practice this can be quite difficult as there are only 15 categories specified plus one "Others" (IC 15/0) for branches that cannot be classified directly. It should be noted that industrial category 5 "Personal/domestic" almost matches the life cycle stage private use. Often

it is difficult to classify the use area. Take for example a substance that is used as a solvent at paint spraying for motorcars. It is possible that the substance is used in the paint formulation, which means that the industrial category should be 14 "Paints, lacquers and varnishes". Another possibility is that the substance is used as a diluent at paint spraying. As the spraying of motorcars is involved there can be spraying in motorcar industry or in the automotive repair industry. The use in motorcar industry is likely to be classified in industry category 16 "Engineering industries: civil and mechanical". This use takes place at large point sources. The use in the automotive repair industry is usually carried out by professionals at a much smaller scale. It is likely that industrial category 15/0 "Others" will be chosen or even industrial category 6 "Public domain".

Sub 3

The use category reflects the purpose or the function of the substance but can also point at the real use, which normally than has a direct link to the industrial category. The 55 use categories of the TGD have a varying level of detail and are often very difficult to determine by the notifier making the selection of the right identifier very difficult and confusing. Furthermore, use categories are often integrated in the emission scenarios, where the use categories may have specific emission factors.

Sub 4

The details on the envisaged use of the substance usually reveal clearly the industrial area or process (industrial category) where the substance - or a preparation containing the substance - is used. From these data it will also become evident what kind of preparations with the substance will be of importance giving adequate information on identifiers.

It should be noted that for the two exemplified branches in this report data according to the present situation - i.e. notification of a new substance - have been considered.

2.1.1 Information in Emission Scenario Documents (ESDs)

An ESD contains one or more emission scenarios and each emission scenario can be subdivided into one or more emission estimation modules (EEMs). The emission scenarios in the ESDs of the TGD and of the OECD are varying in level and detail. In principle they may vary from a scenario for a single process (so, one stage of the life cycle) concerning a single specific function and just one receiving environmental compartment to a scenario for a whole industry branch - or even industrial category of the TGD - for all types of functions of substances including biocides and all environmental compartment and stages of the life cycle.

Another complicating factor is the fact that the use category or the function specified in the detailed description on envisaged use may concern different stages of the life cycle.

2.2.2 Classification of processes and activities

The TGD employs 16 industrial categories (ICs; for an overview see Figure 9). The determination of these industrial categories is often difficult for more reasons than discussed in section 2.1. In one IC many different processes may occur for which specific emission scenarios will be needed. And in quite a number of cases a process occurs in various ICs. An example is degreasing and cleaning. Though the process is the same the size of the process varies depending upon the industrial activity. For economical statistics classification systems are used, in the EU NACE (Nomenclature générale des Activités économiques dans les Communautés Européennes) and in Canada, Mexico and the USA NAICS (North American Industrial Classification System). Especially for the size of point sources statistical data collected for industrial branches might be important in the development of ESDs. Therefore, one of the elements of the project A was to investigate the possibility to use NACE/NAICS codes and specific processes for the OECD matrix project. So far no workable system could be developed in the time available (see Chapter 4). However, an idea for a design is presented in Annex 4. As a basis for this idea only the NACE codes have been used. However, it is is expected that combination of NACE and NAICS codes will not be too problematic. Actions have been undertaken already to streamline the two systems.

2.2.3 Examples

In order to show the various aspects involved in the proper selection of identifiers which lead to the appropriate emission estimates, a few examples will be discussed in detail. The examples concern imaginary substances used in paint applications and regarding their function and life cycle stage an overview is given in Figure 3.

Example 1 (left hand scheme in Figure 3)

In two separate notifications the notifier states that one substance is used as an in-can preservative (use category 39 "Biocides, non-agricultural") for water-based paints or that the other substance is used during paint manufacturing as a dispersing agent (possible use categories 43 "Process regulators" and 50 "Surface-active agents"). The preservative serves as a performance additive, which prolongs the shelf-life of the paint product. The dispersing agent serves as a processing aid during paint manufacturing. In both cases the substances are used during the life cycle stage "formulation". At application of the paint the substance has no function anymore but will remain in the paint, also after drying, and then will enter the life cycle stages service life and waste treatment.

It should be noted that the application as a processing aid at formulation might be considered also as the stage of the life cycle "industrial use". However, because the substance remains in the chemical product (paint) the life cycle for this preparation with the substance in it is followed in that case.

A performance additive like the preservative in this example has the task to keep the chemical product (paint) in good order in the period between manufacturing and use. Therefore, it has been integrated in this scheme as a part of the life cycle stage formulation.

Example 2 (mid schemes in Figure 3)

This example concerns two substances that are used as a processing aid at paint application, i.e. life-cycle stage industrial use (professional use or private use, respectively). The first substance is a solvent (use category 48 "Solvents") used as a diluent for paint spraying. The use of a solvent as a diluent can be in two ways. First, the solvent can be used at the manufacture of the paint, i.e. in the life cycle stage formulation. Second, the solvent can be used at application of the paint in order to ensure the proper viscosity, i.e. in the life cycle stage industrial use. In this case the

substance will not remain in the paint layer after drying. The possibility that the substance is not formulated is represented in the scheme by the arrow bypassing this life cycle stage.
The second substance, a processing aid like for example a siccative (UC 43 "Process regulators") will be added during manufacture of the paint (life cycle stage formulation) and remain in the dried paint layer (life cycle stages service life and waste treatment).

Example 3 (right-hand scheme in Figure 3)
In this example an antistatic agent is used as a performance additive in paint. Its action is required in the dried paint layer, i.e. during the life cycle stage “service life”.

Beside the information of the examples some other aspects to be considered are:

- The first stage of the life cycle, i.e. production, is not always relevant as chemicals may solely be imported.
- Sometimes, a substance is formulated into preparations in two subsequent formulation stages. For example, a substance may be formulated into an additive package, which is then formulated into a chemical product like paint.
- The life cycle stages service life and waste treatment (recovery, reuse, incineration, and dumping) do not need special identifiers. Selection of applicable emission scenarios for service life and/or waste treatment will follow automatically from preceding steps in the decision tree. If, for example, a substance is used in printing ink there will be the stage of recycling for paper because the ink with a substance in it will be present on paper ending up as wastepaper.

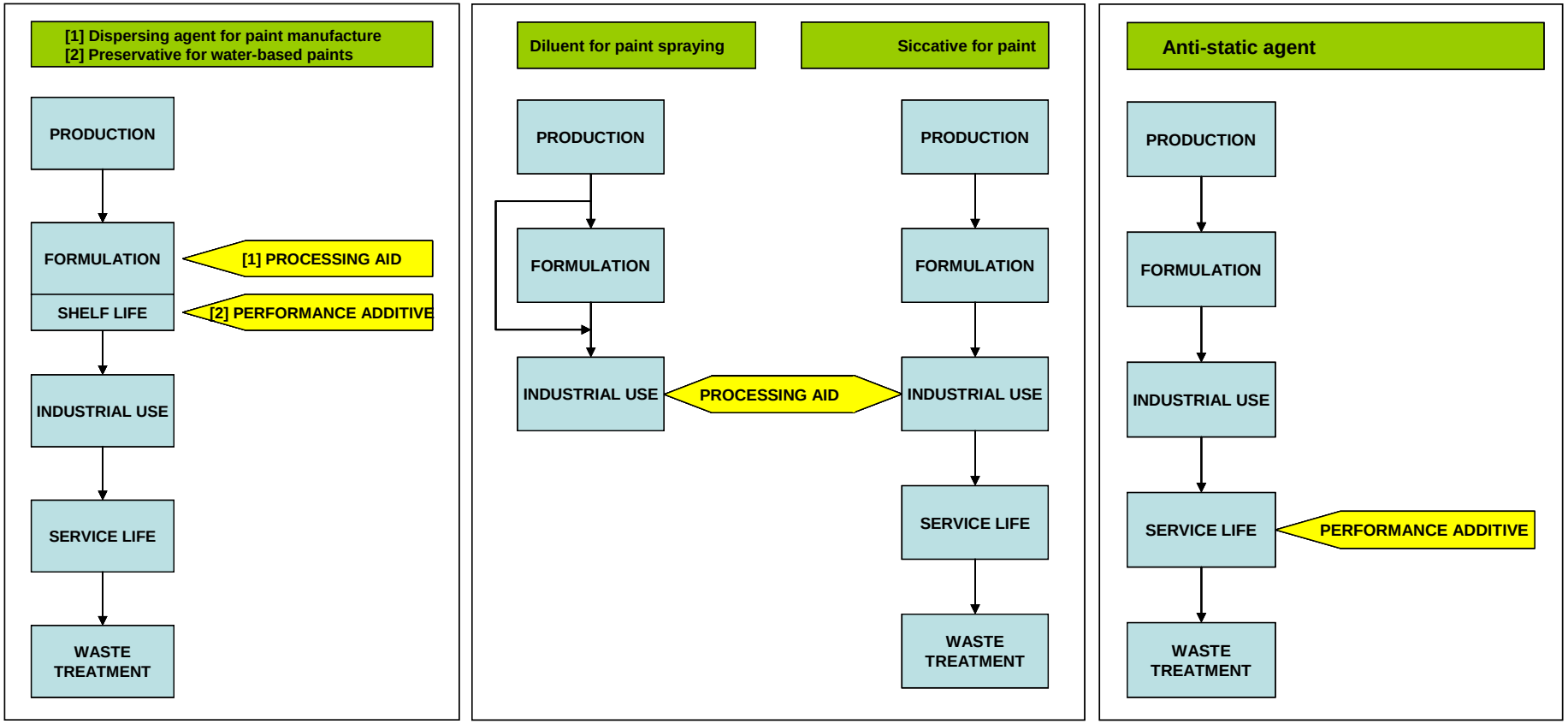

Figure 3 Examples of stages of the life cycle where the substance has its desired purpose for some imaginary substances applied in paint (see text for explanation).

2.3 Target funnel operation and decision tree structure

Altogether, a varying range of data on types of preparations, applications, processes, and stages of the life cycle concerned is required for the selection of the emission scenarios. Because of all possible variations the selection process with the target funnel has to proceed according to a well-defined range of questions, which are incorporated in a decision tree. This is necessary, as not always the same identifiers are needed and cannot be evaluated at the same time.

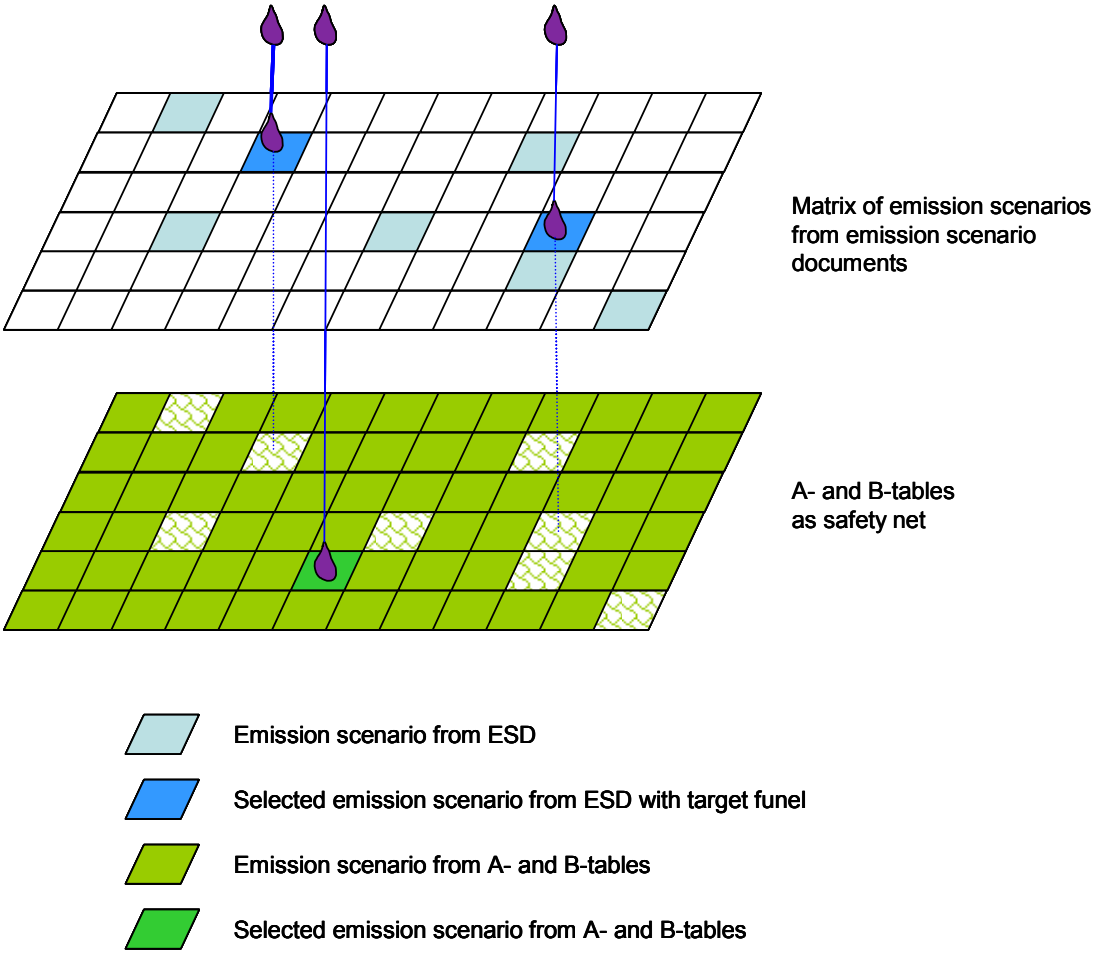

Figure 4 Schematic presentation of the selection of emission scenarios with the target funnel from the matrix with scenarios from ESDs and the scenarios of the A- and B-tables, which serve as a safety net.

If available, emission scenarios derived from emission scenario documents are preferably used. At this moment, there are only a rather limited number of emission scenario documents available. So, the matrix will have to be filled in future with the

development of new emission scenario documents. If such scenarios are not available the scenarios of the A- and B-tables of the TGD are used as a kind of safety net. This approach is schematically presented in Figure 4. It shows the selection of emission scenarios with the target funnel (see Figure 2) by drops falling on a sieve with blocked meshes of (partly) available emission scenarios from ESDs. If there is no emission scenario present the drop passes through the sieve and falls on the scenario of the A- and B-tables. In case A-tables and/or B-tables are used additional identifiers are often required.
As the target funnel is a virtual one, it is impossible to enter all identifiers needed at the same time. Therefore, the target funnel is operated as a kind of decision tree, which might be transformed into a computer program in due time.

In the development of the decision tree the emission scenario documents on photochemicals and plastics additives have especially been analysed. Special attention was given to the various stages of the life cycle (see Figure 1).
For the life cycle stage formulation two types of formulations are distinguished:

(1) semi-finished preparations and

(2) chemical products.

Semi-finished preparations are formulated into chemical products, but might be used as such in a process directly as well. Chemical products are ready-for-use preparations for particular purposes (paints, inks, adhesives etc.). In many branches of industry semi-finished preparations are called additive packages or performance packages.
Figure 5 presents a provisional overview of the identifiers used in pick lists for the two formulation types defined so far. Some types of preparations may be used in more than one product group.

Label	Identifier 4: Semi-finished preparation [1)]
SP1	Dye preparations
SP2	Dyeing auxiliaries (for textile processing)
SP3	Finishing materials (for textile processing)
SP4	Fragrance composition (perfume composition)
SP5	Fuel additives packages
SP6	Lubricant additive packages
SP7	Paint additive packages
SP8	Pigment paste
SP9	Pretreatment agents (for textile processing)
SP10	Surfactant packages

[1)] *Synonyms: Additive package, Performance package*

Label	Identifier 6: Chemical product
CP1	Antifreezes
CP2	Adhesives, glues, sealants
CP3	Biocidal products
CP4	Car maintenance products
CP5	Cleaning products, detergents, soaps
CP6	Cleaning products, solvent-based
CP7	Coating products (paints, lacquers, varnishes)
CP8	Cosmetic products
CP9	Fuels
CP10	Galvanic preparations
CP11	Heat transferring preparations
CP12	Hydraulic fluids
CP13	Leather dyes
CP14	Leather care products
CP15	Leather finishing products
CP16	Lubricants and greases
CP17	Metalworking fluids
CP18	Paper chemicals
CP19	Paper dyes
	Photochemicals, photographic materials
CP20	- for photographic bath
CP21	- photographic materials (e.g. films)
CP22	Plastic compounds (masterbatches)
	Polishes
CP23	- metal polishes
CP24	- floor polishes and waxes
CP25	- wood polishes and waxes
CP26	Semiconductors
CP27	Textile dyes
CP28	Textile care products (? CP5 & CP6)
CP29	Textile coatings
CP30	Textile finishing products
CP31	Toners

Figure 5 Provisional overview of identifiers used in picklists for semi-finished preparations and chemical products (life cycle stage formulation; labels SP and CP)

3. Results

3.1 The decision tree of the target funnel

In this section the general outline of the decision tree, which is presented in Figure 6a and 6b, is elucidated. As it is a decision tree that works top-down the user has to start at the beginning stripping irrelevant sections by appropriate answers to the various questions. Stepwise, the questions and answers, the identifiers and various aspects for each life cycle stage will be discussed in detail below.

Production

The first question asked is if the life cycle stage production has to be assessed. For the life cycle stage production the only emission scenarios covered in ESDs at this moment are for:

1. intermediates (TGD Chapter 7: ESD IC 3 "Chemical industry: chemicals used in synthesis" for UC 33 "Intermediates" at HPVC level in respect of releases into wastewater);
2. substances for soaps, fabric washing, dish washing, and surface cleaning products (TGD Chapter 7: ESDs IC 5 "Personal/domestic" and IC 6 "Public domain" for UC 9 "Cleaning/washing agents" and UC 15 "Cosmetics" at HPVC level).

In all other cases - including the LPVC level for the substances covered in the ESDs for the production stage - the A-tables are used. As there is a specific A-table for dyes used in IC 7 "Leather processing industry", IC 12 "Pulp, paper and board industry", and IC 13 "Textile processing industry" the decision tree has a specific branch for UC 10 "Colouring agents". It should be noted that the source size and time aspect is not covered in the ESDs concerned. So, the B-tables have to be always used.

In Annex 1 the emission tables for the life cycle stage production are presented in relation to the parameters (identifiers) industrial category, use category, production level, and possibly function description. The function description is more or less the same as the use category, but at a more detailed level. It should be noted that the industrial category for the stage of production is the same as for the life cycle stage industrial/professional/private use.

First, the use category has to be chosen from a picklist (identifier 1). This picklist does not contain the complete list of 55 use categories of the TGD. It only contains those use categories for which specific A- and B-tables are provided (see Figure 7 and Annex 2). For dyes used for dyeing leather (IC 7), paper (IC 12), and textile (IC 13) specific A- and B-tables have been provided. Therefore, the specific type of colouring agent has to be chosen from a second picklist (Figure 8) if UC 10 is selected.

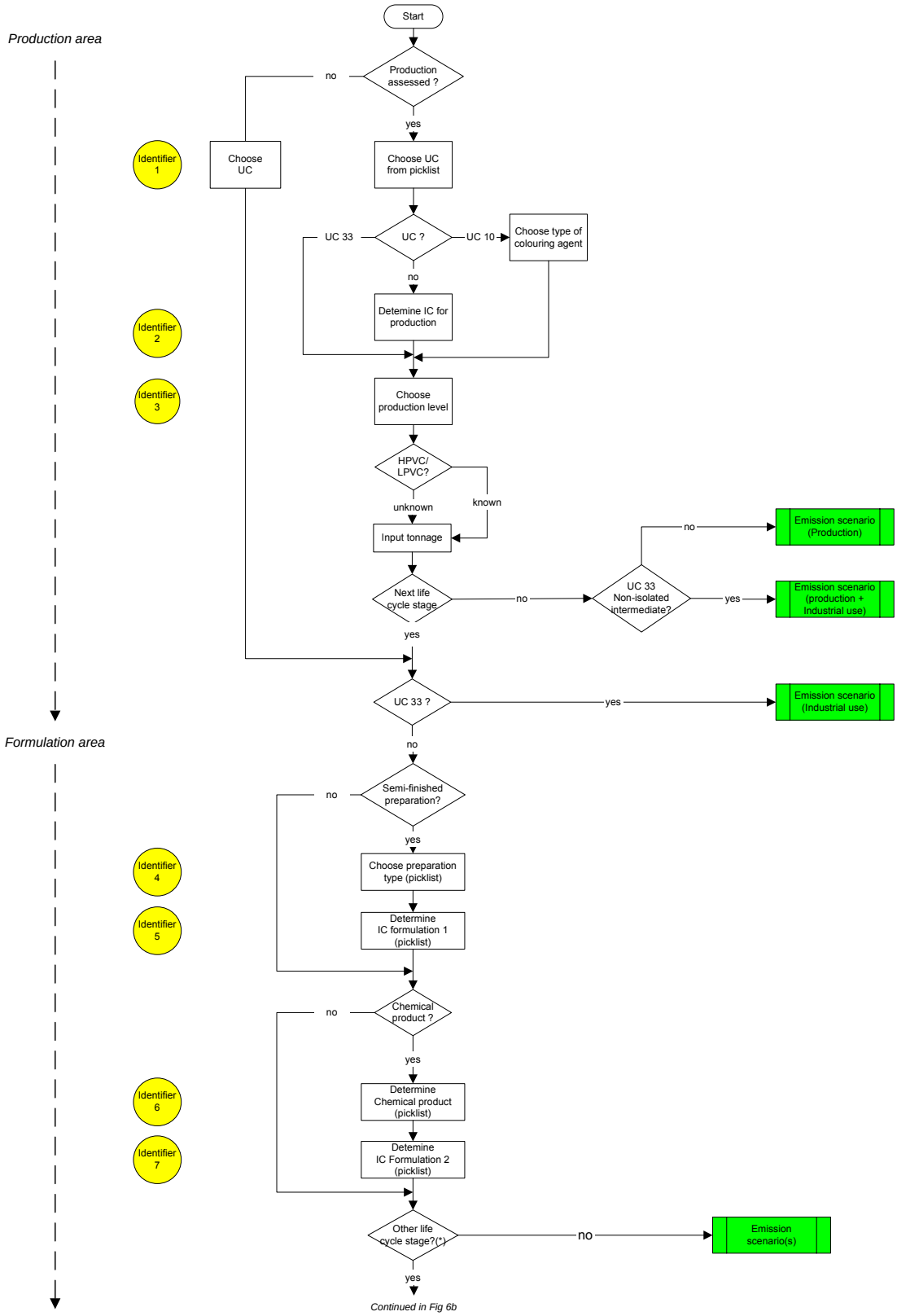

Figure 6a First part of the general outline of the decision tree for selection of emission scenarios for the relevant life cycle stages of a substance; (*) if no other life cycle stage have to be assessed the selected emission scenarios are presented.

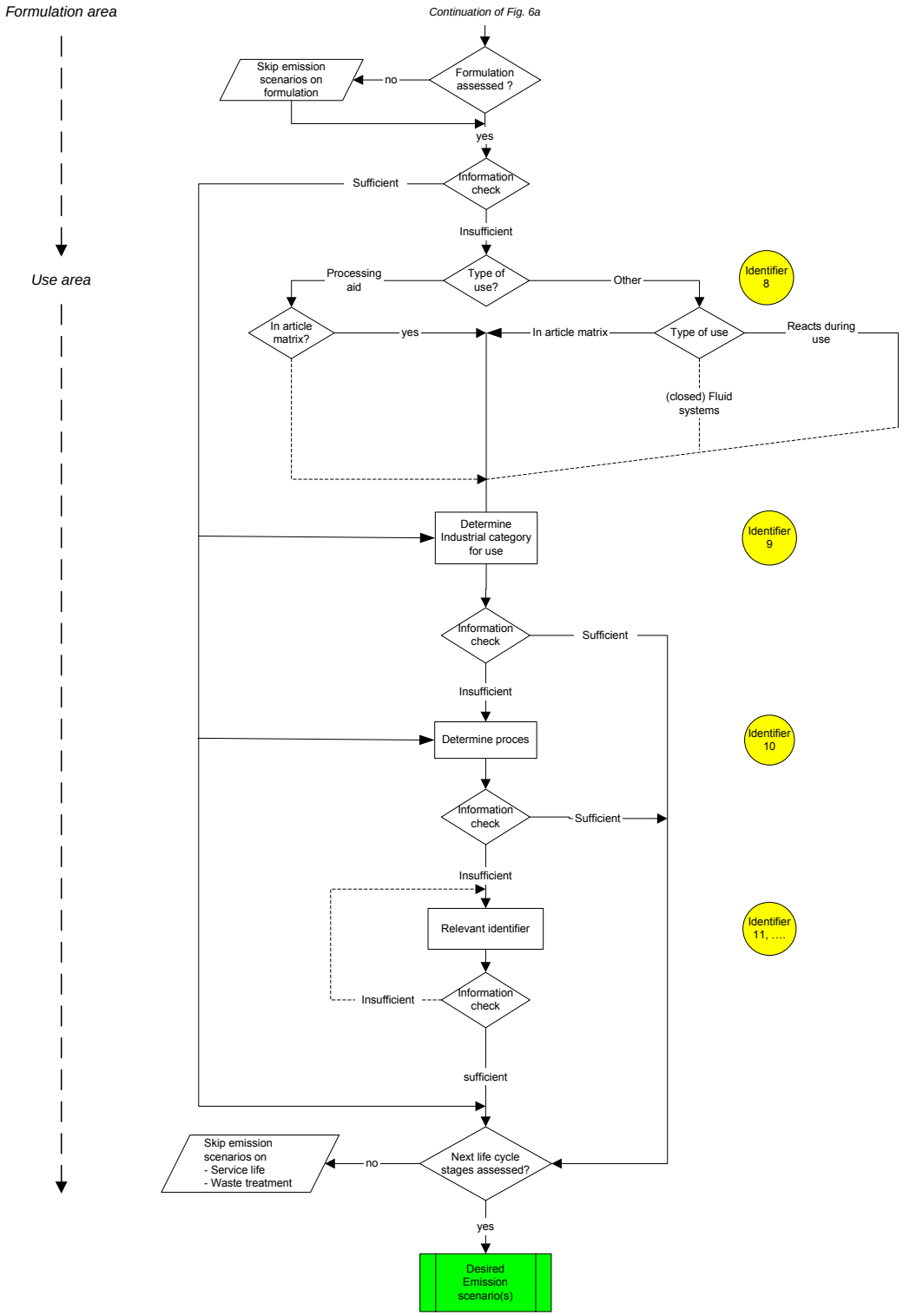

Figure 6b Second part of the general outline of the decision tree for selection of emission scenarios for the relevant life cycle stages of a substance

Next, the industrial category for the production stage has to be chosen from the picklist with the 16 industrial categories of the TGD (identifier 2, see Figure 9). In case of a specific choice for the use category the most likely industrial category should be highlighted. This is shown in Figure 7 - 9 for an example of a colouring agent used for dyeing textiles. This implies the choice of UC 10 "Colouring agents" (picklist of Figure 7) and the choice "textile dyes" for IC 13 (picklist of Figure 8).

Label	Picklist Identifier 1: Use category
UC6	Anti-set-off and anti-adhesive agents
UC9	Cleaning/washing agents
UC10	Colouring agents
UC15	Cosmetics
UC20	Fillers
UC27	Fuels
UC29	Heat transferring agents
UC31	Impregnation agents
UC33	Intermediates
UC35	Lubricants and additives
UC38	Plant protection products, agricultural
UC41	Pharmaceuticals (veterinary medicines)
UC43	Process regulators
UC45	Reprographic agents
UC47	Softeners
UC15/0	OTHERS

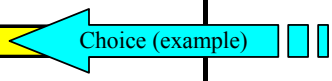

Figure 7
Picklist for the selection of use categories of the TGD for the stage of production (label UC; choice UC 10)

Label	Picklist for UC 10 (Identifier 1)
CA1	Leather dyes
CA2	Paper dyes
CA3	Textile dyes
CA4	*Combination of CA1 - CA3*
CA5	Other dyes
CA6	Pigments
CA7	Others/Unknown

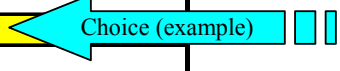

Figure 8
Picklist for the type of colouring agent (label CA; choice textile dyes)

Label	Picklist Identifier 2: Industrial category (production)
IC1	Agricultural industry
IC2	Chemical industry: basic chemicals
IC3	Chemical industry: chemicals used in synthesis
IC4	Electrical/electronic industry
IC5	Personal/domestic
IC6	Public domain
IC7	Leather processing industry
IC8	Metal extraction, refining and processing industry
IC9	Mineral oil and fuel industry
IC10	Photographic industry
IC11	Polymers industry
IC12	Pulp, paper and board industry
IC13	**Textile processing industry**
IC14	Paints, lacquers and varnishes industry
IC16	Engineering industries: civil and mechanical
IC15/0	Others

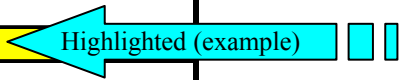

Figure 9 Picklist for the industrial category of the life cycle stage production (label IC; IC 13 highlighted because of choice for textile dyes in previous step).

As for the stage of production different B-tables are used for low production volume chemicals and high production volume chemicals choice between these two tables has to be made. Therefore, identifier 3 "production level" is used. In case the user does not know the tonnage level HPVC or LPVC and chooses "unknown" the tonnage - i.e. the production volume in tonnes per year - has to be entered. The production level is then set on account of the default for the industrial category concerned.
Substances with UC 33 "Intermediates" have a special place. Intermediates are produced to serve as raw materials in the synthesis of particular substances (and products). Usually they are isolated and used later on at the same or another site. However, some intermediates are converted in the same reactor directly without isolation (non-isolated intermediates). So, the production and use stages are combined, which is reflected in the decision tree (Figure 6a) by the emission scenario production + industrial use.

Formulation

Next, the decision on the life cycle stage formulation has to be made. First, there is the choice for a semi-finished preparation (identifier 4). The choice for the type of preparation is made from the picklist shown in Figure 10. On account of the specific use category chosen in the section on production the most likely preparation type might be highlighted.
For this formulation stage the industrial category has to be determined (identifier 5) with the aid of a picklist. This picklist is the same as for the production stage, i.e. the 16 industrial categories of the TGD (see Figure 9). On account of the choice for the semi-finished preparation one or more ICs might be highlighted as the most appropriate ones.

Label	Identifier 4: Semi-finished preparation [1)]
SP1	Dye preparations
SP2	Dyeing auxiliaries (for textile processing)
SP3	Finishing materials (for textile processing)
SP4	Fragrance composition (perfume composition)
SP5	Fuel additives packages
SP6	Lubricant additive packages
SP7	Paint additive packages
SP8	Pigment paste
SP9	Pretreatment agents (for textile processing)
SP10	Surfactant packages

[1)] *Synonyms: Additive package, Performance package*

Figure 10 Picklist for the choice of semi-finished preparations (label SP).

Next the choice for the type of chemical product (identifier 6) can be made in the same way. The picklist is shown in Figure 11. Because of choices for the use category at the production stage and/or for the type of semi-finished preparation one or more of the most likely chemical products might be highlighted. Just as for the semi-finished

preparation the industrial category for the formulation of the chemical product (identifier 7) has to be determined.
In case the substance is not formulated a jump to the life cycle stage for the use (industrial use, professional use or a private use) of the substance is made.
At this moment there are nearly no emission scenario documents with emission scenarios concerning formulation of chemical products and other preparations. Therefore, the A- and B-tables for the same industrial category where the use of the substance will be specified has to be chosen. In future, emission scenarios on formulation might be added if certain emission scenario documents are developed. It should be noted that in future probably specific subcategories might be introduced when ESDs become available for particular types of formulations. The US EPA, for example, presented a new project proposal for an ESD on the formulation of adhesives at the meeting of the OECD Task Force on Environmental Exposure Assessment in September 2004.

Label	Identifier 6: Chemical product
CP1	Antifreezes
CP2	Adhesives, glues, sealants
CP3	Biocidal products
CP4	Car maintenance products
CP5	Cleaning products, detergents, soaps
CP6	Cleaning products, solvent-based
CP7	Coating products (paints, lacquers, varnishes)
CP8	Cosmetic products
CP9	Fuels
CP10	Galvanic preparations
CP11	Heat transferring preparations
CP12	Hydraulic fluids
CP13	Leather dyes
CP14	Leather care products
CP15	Leather finishing products
CP16	Lubricants and greases
CP17	Metalworking fluids
CP18	Paper chemicals
CP19	Paper dyes
	Photochemicals, photographic materials
CP20	- for photographic bath
CP21	- photographic materials (e.g. films)
CP22	Plastic compounds (masterbatches)
	Polishes
CP23	- metal polishes
CP24	- floor polishes and waxes
CP25	- wood polishes and waxes
CP26	Semiconductors
CP27	Textile dyes
CP28	Textile care products (≠ CP5 & CP6)
CP29	Textile coatings
CP30	Textile finishing products
CP31	Toners

Figure 11
Picklist for the choice of chemical products (label CP).

After the section on formulation the user is asked if the next life cycle stage has to be assessed. If this is not case the relevant emission scenarios will be presented. Otherwise, if formulation is not assessed emission scenarios on formulation will be skipped for the report that will be presented after the following life cycle stages.

Use

The life cycle stage use comprises industrial use, professional use, and private use. In most cases the use of the substance - as such or in a formulation - occurs in a specific process, for example painting of houses and paint spraying at motor car refinishing. Such a process is usually one of a large number of different processes within one particular industrial category. In a limited number of cases nearly all processes are covered in one ESD for a whole industrial category. This is the case for IC 13 "Textile processing industry" for example. Often an ESD covers just one process or even one type of substance application in a single process. Examples are the use of the chemical product metalworking fluids at metal processing in IC 8 "Metal processing industry" and the application of substances with the function photoresists in one of the steps in the manufacture of semiconductors. Depending on the information obtained in the sections on production and formulation, a direct jump can be made in the determination of the industrial category for use or of the particular process. It is even possible that the information is already sufficient to determine the relevant emission scenarios already at this stage. If the test on the information obtained is not sufficient the user is asked on the type of use. The types of use as described above are considered as identifier 8 and the choice is made from a picklist (see Figure 12).

Picklist Identifier 8: Type of use		Label
Processing aid	Not in article matrix	TU1
	In article matrix (unintended)	TU2
Other	In article matrix	TU3
	Reacts during use	TU4
	Fluid systems (closed)	TU5

Figure 12
Picklist for the type of use (label TU)

Substances used as a processing aid are not intended to become part of the article matrix. This means that the substances will be emitted and/or end up in waste streams. For example, a detergent used for dishwashing is discharged into the sewer directly after the cleaning process. However, there is a possibility that a substance becomes part of the article matrix, which implies that the life cycle stage service life is involved. An example is a stabiliser for plastics, which protects the polymer from heat degradation during processing. Other types of use can lead to the following three situations. First, the substance can become part of the matrix of an article. Examples are additives for plastics protecting them from degradation or in the colouration during service life of the articles. Second, the substance (as such or in a preparation)

can react during use and, hence, becomes consumed or converted into another substance. Examples are substances used in or as a hardener for epoxy adhesives and (organic) substances present in a fuel. Third, substances - as such or in a preparation - can be used in fluid systems, which can more or less be considered as close systems. Examples are a hydraulic fluid used in aeroplanes and motor oils for cars.

The information obtained here may be important further along in this section in respect to other relevant identifiers needed for the determination of the corresponding emission scenarios and for the relevance of the life cycle stages service life and waste treatment (especially such processes as recycling, recovery, and reuse).
Next, the industrial category (identifier 9) for use has to be determined. If the information obtained so far is not sufficient the process (identifier 10) has to be determined. In metal processing (part of IC 8 "Metal extraction, refining and processing industry") we find amongst others processes like metalworking, cleaning and degreasing, and electroplating. The picklist for this identifier depends upon the industrial category. These picklists have to be developed and will be liable to changes over time. If the information collected now is not sufficient relevant identifiers (identifier(s) 11, 12, . . .) based on the information available will be used. These identifiers are not elaborated up to now.

Service life and waste treatment
At this moment the user will only have to specify whether he wants to assess the next life cycle stages service life (if applicable) and waste treatment (if necessary). The emission scenarios concerned will be clear from the information obtained from any other sections of the life cycle. If the user has indicated that he does not want to assess these life cycle stages the corresponding emission scenarios will be deleted from the final report that is presented. In future specific identifiers might be introduced if emission scenarios for service life and waste treatment become more available.

3.2 Two examples for the application of the decision tree

Two examples of different compounds of a different industrial category, viz. a photochemical and a plastics additive, will be discussed below to illustrate the working of the developed model of a decision tree for the selection of appropriate emission estimates.

3.2.1 Photochemical

For a fictitious photochemical the following information is assumed to be available:

- Production in the EU at the level of 450 tonnes per year;
- The substance is used as in antihalo agent in photographic colour films and as a photochemical it corresponds use category (UC) 42 in the TGD.

Below, the steps of the decision tree with the answers, decisions, and results will be shown and discussed. The substance has to be assessed for all relevant life cycle stages. The following abbreviations are used:

ESD	Emission scenario documents
IC	Industrial category
ID	Identifier
HPVC	High production volume chemical
LPVC	Low production volume chemical
UC	Use category

Item	Decision	Choice	Remarks
Production assessed?	Yes		

ID 1

Use category

Label	Picklist Identifier 1: Use category
UC6	Anti-set-off and anti-adhesive agents
UC9	Cleaning/washing agents
UC10	Colouring agents
UC15	Cosmetics
UC20	Fillers
UC27	Fuels
UC29	Heat transferring agents
UC31	Impregnation agents
UC33	Intermediates
UC35	Lubricants and additives
UC38	Plant protection products, agricultural
UC41	Pharmaceuticals (veterinary medicines)
UC43	Process regulators
UC45	Reprographic agents
UC47	Softeners
UC15/0	OTHERS

As the use category for photochemicals (TGD: UC 42 "Photochemicals") is not present in the picklist the choice "OTHERS" has to be made.

ID 2

Industrial Category

Production

Label	Picklist Identifier 2: Industrial category (production)
. . .	. . . . .
IC9	Mineral oil and fuel industry
IC10	Photographic industry
IC11	Polymers industry
. . .	. . . . .

Item	Decision	Choice	Remarks
ID 3			No information available
Production level		Label: Picklist Identifier 3: Production level PL1 High production volume chemical PL2 Low production volume chemical PL3 Unknown	
Tonnage		Input for Identifier 3: Tonnage 4 5 0 tonnes/year	The tonnage of 450 tonnes per year is filled in. The data entered is used for the determination whether the substance is an LPVC or a HPVC.
Next life cycle stage?	Yes		
Semi-finished preparation?	No		
Chemical product?	Yes		
ID 6		Label: Identifier 6: Chemical product . . . . . . CP19 Paper dyes Photochemicals, photographic materials CP20 - for photographic bath CP21 - photographic materials (e.g. films) CP22 Plastic compounds (masterbatches)	

Item	Decision	Choice	Remarks
ID 7			
Industrial category Formulation			IC 10 might be highlighted as the most likely choice because of the previous choices.
Next life cycle stage?	Yes		
Formulation assessed?	Yes		
<< INFORMATION CHECK >>			From the information on the type of chemical product plus the information on the industrial category for formulation the jump is made to the determination of the process.
ID 10			A help screen should elucidate that wholesale finishers should be chosen. The picklist "Process" is deduced from the ESD. The ESD distinguishes the four categories; the category "Unknown/other" corresponds with IC 10 "Photographic industry".
<< INFORMATION CHECK >>			

Label	Picklist Identifier 7: Industrial category (formulation)
. . .	. . . . .
IC9	Mineral oil and fuel industry
IC10	Photographic industry
IC11	Polymers industry
. . .	. . . . .

Label	Picklist Identifier 10: Process
PR1	Wholesale finishers
PR2	X-ray divisions at hospitals
PR3	Large printing offices for reprographic activities
PR4	Copying facilities (cine & TV)
PR5	Unknown/Other

Next life cycle stages assessed? Yes

The respective emission scenarios for the relevant life cycle stages industrial use and waste treatment are deduced from the chosen identifiers of the previous life cycle stages.

Presentation of results:

Emission scenarios* example "photochemical"			
Life cycle stage	Source	Table 1	Table 2
Production	TGD	A 1.1	B 1.12
Formulation	TGD	A 2.3	B 2.3
Industrial use	ESD 10	EEM 10.2	-
Waste treatment	ESD 10	EEM 10.3	-

*No. of the ESDs and EEMs are taken from project part B

3.2.1.1 Link to computer program

The decision tree as treated in the previous subsection may be written in a different form as presented in Table 1. This table presents the choices for the identifiers and the labels connected to the choices, which help to find the correct emission scenarios in Table 2. Table 2 gives the overview of all emission scenarios/EEMs that might be applicable for photochemicals. This table might be helpful in the development of an automated IT system (computer program).

As can be seen from this example use category 42 "Photochemicals" as specified in the TGD is not used as an identifier. It will be useful to elaborate an extended list with functions that substances can have in a lot of processes and products. In the case of photochemicals - use category 42 in the TGD - there will be a whole list of functions that substances can have in the various processing baths and photographic materials. Some of these functions will occur in the TGD with a use category, but many will not. It should be noted that the use category can be used as a relevant identifier (identifier 10 . . .) in some cases. However, in many ESDs the use category – or more precisely the exact function – of the substance is used within the emission scenarios themselves (so, after the determination of the emission scenarios).

Table 1 Layout for programming the decision tree in case of photochemicals; the values of the choices determine the correct emission scenarios in Table 2. Gray fields present alternative choices that are not relevant for the example substance.

Identifier		Choice	Label	Elucidation
1	Use category	Others	UC15/0	No specific label needed for the stage of production
2	Industrial category (production)	IC 10 Photographic industry	IC10	Other possible choices not shown here
3	Production level	LPVC	PL1	
		HPVC	PL2	
		Unknown	PL3	*Go to 3b*
3b	Tonnage	< 4000 tonnes/year	PL1	Identifier 3 Production level = LPVC
		≥ 4000 tonnes/year	PL2	Identifier 3 Production level = HPVC
4	Preparation type			Not applicable
5	Industrial category (formulation)			Not applicable
6	Chemical product	Photographic materials	CP21	Other possible choices not shown here
7	Industrial category (formulation)	IC 10 Photographic industry	IC10	Other possible choices not shown here
10	Process	Wholesale finishers	PR1	
		X-ray decisions at hospitals	PR2	
		Large printing offices for reprographic activities	PR3	
		Copying facilities (cine & TV)	PR4	
		Unknown/Other	PR5	

Table 2 Overview of all possible emission scenarios for photochemicals; the labels for the identifiers of Table 1 determine the selection of the correct emission scenarios.*

Life cycle stage	Identifier	Label	Identifier	Label	Source	Table 1	Table 2
Production	Production level	PL1	-		TGD	A 1.1	B 1.12
		PL2			TGD	A 1.1	B 1.4
Formulation	Production level	PL1	Chemical product	CP1	TGD	A 2.1	B 2.8
		PL2		CP1	TGD	A 2.1	B 2.3
		PL1		CP2	TGD	A 2.3	B 2.8
		PL2		CP2	TGD	A 2.3	B 2.3
Industrial use	Process	PR1-PR4	Chemical product	CP20	ESD 10	EEM 10.1	
				CP21	ESD 10	EEM 10.2	
		PR5	-		TGD	A 3.9	B 3.8
Private use	-		-		TGD	A 4.3	B 4.2
Service life					*Not covered*		
Waste treatment:							
- recovery	Chemical product	CP20	-		ESD 10	EEM 10.3	
		CP21			*Not covered*		
- waste streams		CP21			*Not covered*		

*No. Of the ESDs and EEMs are taken from project part B

3.2.2 Plastics additive

For a fictitious plastics additive the following information is assumed to be available:

- The substance is imported into the EU at the level of 450 tonnes per year.
- The substance is used as a colouring agent in plastics.
- All relevant life cycle stages have to be assessed.

Notes:

The importer should know about the use of the pigment in pigment pastes (preparation) and masterbatches (chemical product). It is assumed here that these formulation stages do occur as this is very likely.

From the emission scenario document for IC 11 "Polymers industry" it appears that the formulation of masterbatches also occurs at sites where polymer processing takes place; pigment pastes can be applied here directly at polymer processing, which represents the life cycle stage industrial use. So, in this case the life cycle stage is covered at the same time then. The decision tree should offer the possibility to choose between formulation of masterbatches exclusively and both formulation and industrial use. This has been worked out in the example presented here.

Below, the steps of the decision tree with the answers, decisions, and results will be shown and discussed. The following abbreviations are used:

ESD	Emission scenario documents
IC	Industrial category
ID	Identifier
HPVC	High production volume chemical
LPVC	Low production volume chemical

Item	Decision	Choice	Remarks
Production Assessed?	No		Substance imported into EU
Next life cycle stage?	Yes		
Semi-finished preparation?	Yes		

ID 4
Semi-finished preparation

Label	Identifier 4: Semi-finished preparation [1)]
SP1	Dye preparations
SP2	Dyeing auxiliaries (for textile processing)
SP3	Finishing materials (for textile processing)
SP4	Fragrance composition (perfume composition)
SP5	Fuel additives packages
SP6	Lubricant additive packages
SP7	Paint additive packages
SP8	Pigment paste
SP9	Pretreatment agents (for textile processing)
SP10	Surfactant packages

[1)] *Synonyms: Additive package, Performance package*

ID 5
Formulation

Label	Picklist Identifier 2: Industrial category (production)
IC1	Agricultural industry
IC2	Chemical industry: basic chemicals
IC3	Chemical industry: chemicals used in synthesis
IC4	Electrical/electronic industry
. . .	. . . . .

Chemical product?	Yes		

Item	Decision	Choice	Remarks
ID 6 Chemical product			It should be noted that both CP7 "Coating products (paints, lacquers, varnishes)" and CP22 "Plastics compounds (masterbatches)" might be highlighted - as presented here in the example - as pigment pastes are used in the manufacture of both of these chemical products.

Label	Identifier 6: Chemical product
CP1	Antifreezes
CP2	Adhesives, glues, sealants
. . .	. . . . .
CP6	Cleaning products, solvent-based
CP7	**Coating products (paints, lacquers, varnishes)**
CP8	Cosmetic products
. . .	. . . . .
. . .	. . . . .
CP22	Plastic compounds (masterbatches)
	Polishes
CP23	- metal polishes
. . .	. . . . .

ID 7
IC Formulation 2

Label	Picklist for industrial category	Formulation	Industrial use
IC2	IC 2 Chemical industry: basic chemicals	X	
IC11*A*	IC 11 Polymers industry *Manufacture of masterbatches*	X	
IC11*B*	IC 11 Polymers industry *Manufacture of masterbatches* *+ Polymers processing*		

Identifiers 8 – 9 are skipped

If the application of pigment pastes both in masterbatches and at polymer is processing has been chosen the identifiers 7 - 9 have not to be specified by the user.
It should be noted that manufacture of masterbatches as a single process might be ascribed to IC 2 "Chemical industry: basic chemicals".

Use stage assessed? Yes

Item	Decision	Choice	Remarks
Formulation assessed?	Yes		If the stage of formulation is not assessed the presentation of emission scenarios for formulation will be skipped in the report.
<< CHECK INFORMATION >>			As sufficient information for the life cycle stage industrial use has already been provided previously, (industrial) use with identifiers 8 - 10 is bypassed.
Next life cycle stages assessed?	Yes		If the stages service life and waste treatment are not assessed (answer "No" to the question) the emission scenarios for the stages will not be presented in the final report. Sufficient information for the selection of the emission scenarios in these life cycle stages are already given in the previous life cycle stages.

Presentation of results:

Emission scenarios example "plastics additive"			
Life cycle stage	Source	Table 1	Table 2
Formulatic - pigment paste	TGD	A 2.1	B 2.4
- masterbatche	OECD 3	EEMs 11.2/11.8 - 11.3/11.9	
Industrial use	OECD 3	-	
Formulation (masterbatches) + Industrial use	OECD 3	EEMs 11.6/11.8 - 11.7/11.9	
Private use	*Not applicable*		
Service life	OECD 3	EEMs 11.12 & 11.13	
Waste tre - recovery	*Not covered*		
- waste streams	OECD 3	EEMs 11.14 & 11.15	

*No. of the ESDs and EEMs are taken from project part B

Remark:

As at a site both formulation of masterbatches and polymer processing may occur a combination of the life cycle stages formulation and industrial use has been introduced in the ESD.

3.2.2.1 Link to computer program

Table 3 presents the the decision tree as treated in the previous subsection in a different form. This table presents the choices for the identifiers and the labels connected to the choices, which help to find the correct emission scenarios in Table 4. Table 4 gives the overview of all emission scenarios that might be applicable. This table might be helpful in the development of an automated IT system (computer program).

Table 3 Layout for programming the decision tree in case of plastics additives (pigment, only imported at the level of 450 tonnes per year); the values of the choices determine the correct emission scenarios in Table 4. Gray fields present alternative choices that are not relevant for the example substance.

Identifier		Choice	Label	Elucidation
1	Use category	UC 10 Colouring agents	UC10	Other possible choices not shown here
1b	Type of colouring agent	Pigments	CA6	Other possible choices not shown here
2	Industrial category (production)	IC 2 Chemical industry: basic chemicals	IC2	
		IC 11 Polymers industry	IC11	➡ choice by the user (other choices but the most
		IC 14 Paints lacquers and varnishes industry	IC14	likely ones are not shown here)
3	Production level	LPVC	PL1	
		HPVC	PL2	
		Unknown	PL3	*Go to 3b*
3b	Tonnage	< 4000 tonnes/year	PL1	Identifier 3 Production level = LPVC
		≥ 4000 tonnes/year	PL2	Identifier 3 Production level = HPVC
4	Preparation type	Pigment paste	SP8	Other possible choices not shown here
5	Industrial category (formulation 1)	IC 2 Chemical industry: basic chemicals	IC2	Other possible choices not shown here
6	Chemical product	Coating products (paints, lacquers, varnishes)	CP7	
		Plastics compounds (masterbatches)	CP22	➡ choice by the user (other choices but the most likely ones are not shown here)
7	Industrial category (formulation 2)	IC 2 Chemical industry: basic chemicals	IC2	
		IC 11 Polymers industry: manufacture of masterbatches	IC11*A*	
		IC 11 Polymers industry: manufacture of masterbatches + polymer processing	IC11*B*	

Table 4 Overview of all possible emission scenarios for plastic additives; the values for the identifiers of Table 3 determine the selection of the correct emission scenarios (Manufacture (i.e. synthesis) of primary polymers not included here).*

Life cycle stage	Identifier	Label	Identifier	Label	Identifier	Label	Identifier	Label	Source	Table 1	Table 2
Production 1)	Use category	UC10	Use (sub)category	CA6	Industrial category	IC2	Production level	PL1	TGD	A 1.1	B 1.1
								PL2	TGD	A 1.1	B 1.2
						IC11		PL1	TGD	A 1.1	B 1.9
								PL2	TGD	A 1.1	B 1.4
						IC14		PL1	TGD	A 1.1	B 1.2
								PL2	TGD	A 1.1	B 1.6
		UC20	Industrial category	IC11	Production level	PL1	-		TGD	A 1.1	B 1.13
						PL2			TGD	A 1.1	B 1.14
		UC43		IC11		PL1			TGD	A 1.1	B 1.13
						PL2			TGD	A 1.1	B 1.14
		UC47		IC11		PL1			TGD	A 1.1	B 1.13
						PL2			TGD	A 1.1	B 1.14
		Others		IC2		PL1			TGD	A 1.1	B 1.1
						PL2			TGD	A 1.1	B 1.5
				IC11		PL1			TGD	A 1.1	B 1.9
						PL2			TGD	A 1.1	B 1.4
Formulation [1]	Preparation type 2) *(pigment paste)*	SP8	Industrial category 3)	IC2	Production level	PL1	-		TGD	A 2.1	B 2.4
						PL2			TGD	A 2.1	B 2.5
				IC11	[UC Production]	UC20, UC43 & UC47	Production level	PL1	TGD	A 2.1	B 2.8
								PL2	TGD	A 2.1	B 2.9
						Other labels		PL1	TGD	A 2.1	B 2.8
								PL2	TGD	A 2.1	B 2.3
Formulation [2]	Chemical product 4)	CP22	Industrial category	IC2 / IC 11	-		-		OECD 3	EEM 11.2/11.8 & 11.3/11.9	
Industrial use	Industrial category	IC11	-		-		-		OECD 3	EEM 11.4/11.8 & 11.5/11.9	
		≠ IC11							TGD	A 3.16	B 3.14
Formulation + Industrial use	Chemical product *(masterbatches)*	CP22	Industrial category	IC11					OECD 3	EEM 11.6/11.8 & 11.7/11.9	
Professional use	*Not applicable*										
Private use	*Not applicable*										
Service life	-								OECD 3	EEM 11.12 & 11.13	
Waste treatment:											
- Recovery	-								*Not covered*		
- Waste streams	-								OECD 3	EEM 11.14 & 11.15	

1) if the substance is not produced in but only imported into the EU the production level is set according to the default for an HPVC for the production stage
2) for the present list of semi-finished there is only one preparation type
3) choices for the industrial category other then IC 2 and IC 11 are not shown here
4) other possible choices are not shown here (e.g. lubricants)

*No. of the ESDs and EEMs are taken from project part B

4. Discussion

The discussion below has been divided into two sections emphasizing and highlighting the various aspects obtained in this study.
Furthermore, a survey was carried out for the practicability of NACE (and NAICS) codes together with industrial categories for the target funnel. At this moment the use of NACE codes has little relevance.

4.1 Parameters for identifiers

4.1.1 Selection of identifiers

In general, the data supplied by the notifier will serve to select (find) the appropriate parameters (identifiers).
Regarding emissions and the life cycle of a substance, four important *types of data* can be considered for the selection of identifiers to be used in the decision tree and leading to the appropriate emission scenario.

1 *Physico-chemical properties*. These are important in the emission scenarios, however, they are not applied as identifiers in the tool presented in this report.
2 *Industrial category (IC)*. Supplies information on the area of use or where the substance (as such or in preparation) has to exert its function. In selecting the correct IC for a substance, one must consider (i) that various stages of the life cycle may require different ICs, (ii) the variability of its application, and (iii) the possible occurrence of two consecutive formulation stages. At present only one IC can been specified.
3 *Use category (UC)*. Provides information on the specific use of a substance. However, the selection of the appropriate UC in the decision tree is sometimes difficult because of (i) various applications of the substance, (ii) the limited number of the TGD use categories (55), and (iii) variation in level of UCs.
4 *The envisage used*. Reveals frequently the IC and exact UC of a substance with various applications. The area where the substance (as such or in preparation) is applied is often difficult to determine and the function of the substance in a

certain application is often difficult to translate into one of the 55 UCs of the TGD.

4.1.2 Parameters of emission scenarios documents

Investigating how the ESDs were structured and which parameters would have to be used as identifiers and which parameters - being possible identifiers - were incorporated in them, the following problems were encountered:

- The present ESDs are of a varying level. An ESD may cover: (i) one life cycle stage or all relevant life cycle stages, (ii) one environmental compartment or all relevant ones, (iii) one specific process, a selection or all processes of an industrial branch or industry category, and/or (iv) all functions and uses of the substance or just one specific function.
- Many ESDs cover only emission factors but do not contain data for the amount applied per day. Therefore, B-tables have to be selected.
- One ESDs may require a certain parameter as an identifier, whereas another ESD does not require the parameter at all or uses the parameter internally to differentiate an emission scenario or even within an emission scenario for the selection of specific emission factors.

4.2 The proposed decision tree

As shown by the test with the two examples, the developed decision tree easily leads to the appropriate emission scenario of the involved substance. However, the decision tree might require some changes due to the needs of industry and probably the programmers of an automated version. This will only appear later in time when the decision tree is tested under real conditions. The proposed pick lists are provisional and care should be taken that the system should be flexible and easy to adapt, esp. to the requirements of other branches.

5. Conclusions

5.1 Conclusions connected to the work on the target funnel

The work on the target funnel leads to the following conclusions:

5.1.1. The present structure of data supplied according to the TGD makes it difficult to operate the target funnel as underlying know-how is important.

5.1.2. The present lists of ICs and UCs is inadequate and requires a good knowledge and understanding (see recommendation 2). Often a particular process in which the substance - as such or in a preparation - is applied within an IC has to be known in order to identify the correct emission scenario.

5.1.3. The present ESDs are very different of structure and of way of elaboration, which makes interpretation for the target funnel difficult (see recommendations 6.2.1 and 6.2.2).

5.1.4. The A- and B-tables of the TGD, which serve as a safety net in case there is no ESD, complicate the structure of the target funnel as the requirements of two systems (ESD and A-/B-tables) have to be considered.

5.1.5. In most cases more information will be needed. On account of the information supplied so far, relevant identifiers are used. These identifiers have to be defined on the basis of the available ESDs.

5.1.6. One of the complicating factors is the fact that the function (use category) of the substance can be related to a different stage of the life cycle (see Annex 5).

5.2 Other conclusions

5.2.1. There is no complete matrix of industrial activities, processes, and emission scenarios available now. A first matrix overview over existing information are presented in part B of the project.

5.2.2. As a result of the previous conclusion, there is no good insight in ESDs which might be needed (priorities, emission scenarios applicable for many industrial activities; see also part B of the project).

6. Recommendations

6.1 Recommendations connected to the target funnel

As regards further implementation and development, the following recommendations are given:

6.1.1. The present ESDs of the TGD and OECD should be analysed and necessary modifications and additions to the target funnel realised accordingly.

6.1.2. The provisional lists for semi-finished preparations and chemical products should be amended in cooperation with industry experts.

6.1.3. A flexible interface for an automated version should be designed together with IT experts.

6.2 Other recommendations

6.2.1. Existing ESDs should be updated to a standard format where needed.

6.2.2. Existing ESDs should be updated for missing relevant environmental compartments.

6.2.3. Revision of the industrial categories of the TGD incorporating coding is used in NACE/NAICS resulting in a set of "activities" (industrial branches). This revision should have as a starting point the life cycle stages production (IC 2 "Chemical industry: basic chemicals"), formulation (partly covered by IC 2 "Chemical industry: basic chemicals"), industrial use, professional use (for a part covering IC 6 "Public domain"), private use (IC 5 "Personal/domestic"). See also Annex 4 "Idea for categorisation".

6.2.4. Identification of processes (and eventually process steps) for the new categories for industrial (and other non-industrial) activities, followed by making an inventory of processes occurring in more than one activity (only one ESD needed).

6.2.5. Drawing up a matrix of potential ESDs that could be used for the activities and/or processes identified under 6.2.4.

6.2.6. Priority setting for the potential ESDs of the matrix to be developed. Data on substances that have been notified over the years might be of help.

6.2.7. Application of generic emission scenarios for all low priority activities and/or processes of the potential ESDs. Probably modified A- and B-tables can be used.

6.2.8. Revision of the list of function/use categories together with industry experts. Such a list might consist of "main" categories with subdivisions and synonyms. It would be very useful if the categories are linked to processes in industry (in other words links to the industrial activities).

7. Summary

Because of the huge diversity in applications and functions, the emission estimation is one of the most problematic areas in quantitative risk assessment. Therefore, in this study a tool has been developed for manufacturers, importers, and downstream users of chemical substances. The tool determines the appropriate emission scenarios (emission estimate modules) facilitating emission estimation for wastewater, air, soil and, if possible, solid waste for all relevant functions and life cycle stages, e.g. production and formulation, in all possible applications and processes throughout industry and society.

The crucial part of the tool is the interactive decision tree leading to the required location of a matrix, which contains all information on available emission estimates (modules). The matrix information is based on emission estimation modules derived from existing emission scenario documents of the EU TGD and the OECD and, if not available, default values of the EU TGD (contained in the so-called “A-” and “B-”tables) . The routing through the decision tree is determined by selecting the right parameters (identifiers) for each life cycle stage. The main identifiers, such as the relevant IC and UC, and the type of chemical product or semi-finished preparation (performance package) are overviewed and defined.

The information of this methodology has been structured in such a way that it can easily be implemented into a computer program.

The methodology has been tested and illustrated for two substances in different industrial categories, i.e. a photochemical and a plastics additive, rendering appropriate emission scenarios.

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9. Glossary and definitions

Additive	Substances added to oils, fuels, paint products, food etc., to improve specific properties (e.g. to improve lubricity in oils, and in food [1] to control food texture, [2] to improve nutritional value, [3] to maintain freshness and safety, [4] to rise and to control the acid-base balance, [5] to improve flavour and colour) (http://www.hydrocarbons-technology.com/glossary/additives.html; http://www.northmemorial.com/healthencyclopedia/content/1903.asp; http://www.wordreference.com/definition/additive).
Chemical	[noun] A substance that is produced or used in a process (reaction) involving changes to atoms or molecules. The term is sometimes defined more broadly as "a substance" (See substance; http://www.ilpi.com/msds/ref/chemical.html).
Chemical product	Substance or mixture of substances for particular purpose (e.g. decorating paint, printing ink, toner for photocopying); chemical products may be classified in product groups (e.g. coating products, inks and colours).
Emission	A substance that is emitted or released [syn.: discharged]; in the case of risk assessment, the emission rate is meant, meaning the mass flow expressed as mass per time ($kg.d^{-1}$).
Emission Estimation	Emissions considered during all relevant parts of the life cycle of the substance under the assumption that the risk management measures described in the exposure scenario have been implemented (Annex I of the REACH Regulation, Section 5.2.2).
Emission Estimation Module (EEM)	Equation, often presented with one or more tables with parameters and appropriate defaults, for the calculation of the emission; an ESD consists of one or more EEMs.
Emission scenario document (ESD)	Document containing one or more emission scenarios.
Emission scenario	A description of sources, production processes, pathways and use patterns with the aim of quantifying the emissions (or releases) of a chemical from (1) production,

	(2) formulation, (3) industrial use, (4) professional use (skilled trades), (5) private and consumer use, (6) service life of article/product, (7) recovery, and (8) waste disposal (incineration, landfill) into water, air, soil, and/or solid waste. Remark: Usually one or more equations (EEMs, emission estimation modules) are presented with one or more tables with parameters and appropriate defaults.
Exposure Assessment	The objective of exposure assessment shall be to make a quantitative or qualitative estimate of the dose/concentration of the substance to which humans and the environment are or may be exposed. The exposure assessment shall entail the following two steps: (1) Development of exposure scenarios; (2) Exposure estimation (Annex I of the REACH Regulation, Section 5).
Exposure Estimation	The exposure estimation entails three elements: (1) emission estimation; (2) chemical fate and pathways; (3) estimation of exposure levels (Annex I of the REACH Regulation, Section 5.2.1)
Exposure Scenario (ES)	The set of conditions that describe how the substance is manufactured or used during its life cycle and how the manufacturer controls, recommends downstream users to control, exposure to humans and the environment (Annex 1 of EC, 2003a).
Formulation	[noun] A substance mixture prepared according to a formula (preparation), [verb] mixing and blending of substances into a preparation.
High production volume chemical (HPVC)	Chemicals placed on the EU market in volumes exceeding 1000 tonnes per year per day per manufacturer or importer (EC, 2001).
Industrial categories (IC)	Categories that present industrial use areas for chemicals. Some substances will be used in more than one industrial category. The TGD contains 16 industrial categories (EC, 2003b)
Low production volume chemical (LPVC)	Chemicals placed on the market in volumes between 10 tonnes and 1000 tonnes per year per producer/importer (EC, 2001)

Life cycle (of a substance)	All stages from the synthesis up to recovery and waste treatment after final use of the substance as such or in articles.
Manufacture	The organised action of making of goods and services for sale (http://www.wordreference.com/definition/manufacture). The operation of making wares or any products by hand, by machinery, or by other agency (http://www.brainydictionary.com/words/ma/manufacture187867.html).
Masterbatch	A masterbatch for rubber formulating consisting of a mixture of rubber and one or more additives, such as carbon black, present in high concentrations (http://efunda.intota.com/multisearch.asp?strSearchType=all&strQuery=rubber+masterbatch). Plastic compound which includes a high concentration of an additive or additives. Designed for use in appropriate quantities with the basic resin or mix so that the correct end concentration is achieved. For example, colour masterbatches for a variety of plastics are extensively used as they provide a clean and convenient method of obtaining accurate colour shades (http://www.specialchem4polymers.com/resources/glossary/index.aspx?id=M).
Mixture	[chemistry] A substance consisting of two or more substances mixed together (not in fixed proportions and not with chemical bonding; WordNet ® 2.0, © 2003 Princeton University)
Preparations	Mixtures or solutions composed of two or more substances (Directive 1999/45/EC)
Production	The manufacture of substances in chemical industry by means of synthesis to be used as intermediates, processing aids or in preparations.
Substances	Chemical elements and their compounds in the natural state or obtained by any production process, including any additive necessary to preserve the stability of the products and any impurity deriving from the process used, but excluding any major solvent which may be separated without affecting the stability of the substance or changing its composition (Directive 1999/45/EC) 1).

Supply chain	The way of substances as they move from producer/import are to manufacturer to wholesaler to retailer to consumer
Use categories (UC)	Categories that represent various functional uses of substances; some of them are subdivided into sub-categories, where appropriate. For clarity, exclusions are indicated in some cases (EC, 2003b). The TGD contains 16 industrial categories (EC, 2003b)

Annex 1 A- and B-tables of the TGD

For all industrial categories distinguished in Chapter 5 of the TGD (EC, 2003b) estimates have been generated for:

1. the *emission factors* for the following stages of the life cycles, i.e. (1) production, (2) formulation, (3) industrial use, (4) private use, (5) professional use, (6) service life, and (7) waste treatment. When possible defaults occurring in emission scenario documents of the TGD have been implemented. All these estimates have been collected in the A-tables.
2. the *fraction of the main source* and the *number of emission days*, which help to estimate the quantity of the substance involved in the operation of the model point source per working day (emission day). These estimates have been collected in the B-tables.

In the development of a quantitative risk assessment system for new substances, emission tables were developed in the Netherlands for a limited number of applications. The applications considered were textile dyes, photochemicals, metalworking fluids, hydraulic fluids, paper chemicals, and intermediates. For these applications so-called use category documents were available. Nearly at the same time a priority setting system for existing chemicals was developed. For this system emission tables were developed for the 15 industrial categories distinguished at that time in the HEDSET (EC/OECD Harmonised Electronic Data Set). The emission factors were established by means of expert judgement and tended to the worst case situation. For the local releases, tables were supplied containing expert judgement for the order of magnitude of the daily amount of the substances for every relevant stage of the life cycle on the basis of the tonnage. The ranges of the tonnages were typical for substances produced in limited amounts. When the TGD and EUSES (European Union System for the Evaluation of Substances) were developed these tables were transformed into what are now referred to as the A- and B-tables (TGD, 2003b and EC, 2004). The A-tables contain emission factors and the B-tables information on the size of operations. They were extended in the following way:

1. extension of the tables with emission factors for several industrial categories. This comprised for example the introduction of main categories or specific use

categories. This was also achieved by expert judgement trying to obtain realistic worst case estimates;

2. insertion of the emission factors of the use category documents mentioned before in the appropriate industrial categories;
3. introduction of B-tables in order to cover higher tonnages for HPVCs (High Production Volume Chemicals). This was also done by expert judgement;
4. new A- and B-tables were developed for the new industrial category 16 "Engineering industries".

Annex 2 Emission scenarios for production

Emission scenarios for the life cycle stage production in relation to conditions for the parameters (identifiers) industrial category, use category, production level, and possibly function description (Part 1)

Industrial Category	Use Category	Production Level	Function Description	Emission Scenarios A- and B-tables		Default Tonnage Production Level
1	38, 41	LPVC	-	A1.1	B1,2	
		HPVC	-	A1.1	B1.4	≥ 3,500
	≠ 38, 41	LPVC	-	A1.1	B1.1	≥ 10,000
		HPVC	-	A1.1	B1.3	
2	-	LPVC	-	A1.1	B1.1	
		HPVC	-	A1.1	B1.5	≥ 10,000
3	≠ 33	LPVC	-	A1.1	B1.2	
		HPVC	-	A1.1	B1.6	≥ 7,000
	33	LPVC	-	A1.2	B1.2	
		HPVC	-	ESD IC3 T1	B1.6	≥ 7,000
4	-	LPVC	-	A1.1	B1.7	
		HPVC	-	A1.1	B1.6	≥ 7,000
5	9, 15	LPVC	-	A1.1	B1.7	
		HPVC	-	ESD IC5/6 T1	B1.6	≥ 1,000
	≠ 9, 15	LPVC	-	A1.1	B1.7	
		HPVC	-	A1.1	B1.6	≥ 7,000
6	9, 15	LPVC	-	A1.1	B1.7	
		HPVC	-	ESD IC5/6 T1	B1.6	≥ 1,000
	≠ 9, 15	LPVC	-	A1.1	B1.7	
		HPVC	-	A1.1	B1.6	≥ 7,000
7	6, 9, 31	LPVC	-	A1.1	B1.9	
		HPVC	-	A1.1	B1.4	≥ 2,500
	10	LPVC	Dyes	A1.3	B1.9	
		HPVC	Dyes	A1.3	B1.4	≥ 2,500
	10	LPVC	≠ Dyes	A1.1	B1.8	
		HPVC	≠ Dyes	A1.1	B1.4	≥ 5,000
	≠ 6,9,10, 31	LPVC	-	A1.1	B1.8	
		HPVC	-	A1.1	B1.4	≥ 5,000
8	29, 35	LPVC	-	A1.1	B1.10	
		HPVC	-	A1.1	B1.4	≥ 2,500
	≠ 29, 35	LPVC	-	A1.1	B1.2	
		HPVC	-	A1.1	B1.6	≥ 7,000
9	27	LPVC	-	A1.1	B1.1	
		HPVC	-	A1.1	B1.11	≥ 25,000
	≠ 27	LPVC	-	A1.1	B1.2	
		HPVC	-	A1.1	B1.4	≥ 3,000
10	-	LPVC	-	A1.1	B1.12	
		HPVC	-	A1.1	B1.4	≥ 4,000

Emission scenarios for the life cycle stage production in relation to conditions for the parameters (identifiers) industrial category, use category, production level, and possibly function description (Part 2)

Industrial Category	Use Category	Production Level	Function Description	Emission Scenarios A- and B-tables		Default Tonnage Production Level
11	20, 47	LPVC	-	A1.1	B1.13	
		HPVC	-	A1.1	B1.14	≥ 60,000
	43	LPVC	Monomers	A1.1	B1.13	
			Cross-linking agents			
			Curing agents			
		HPVC	Monomers	A1.1	B1.14	≥ 60,000
			Cross-linking agents			
			Curing agents			
	43	LPVC	Inhibitors	A1.1	B1.9	
			Initiators			
			Retarders			
		HPVC	Inhibitors	A1.1	B1.4	≥ 3,000
			Initiators			
			Retarders			
	≠ 20, 43, 47	LPVC	-	A1.1	B1.9	
		HPVC	-	A1.1	B1.4	≥ 3,000
12	10	LPVC	Dyes	A1.3	B1.9	
		HPVC	Dyes	A1.3	B1.4	≥ 2,500
	10	LPVC	≠ Dyes	A1.1	B1.8	
		HPVC	≠ Dyes	A1.1	B1.4	≥ 4,500
	45	LPVC	-	A1.1	B1.9	
		HPVC	-	A1.1	B1.4	≥ 2,500
	≠ 10, 45	LPVC	-	A1.1	B1.8	
		HPVC	-	A1.1	B1.4	≥ 4,500
13	10	LPVC	Dyes	A1.3	B1.2	
		HPVC	Dyes	A1.3	B1.6	≥ 7,000
	10	LPVC	≠ Dyes	A1.1	B1.2	
		HPVC	≠ Dyes	A1.1	B1.6	≥ 7,000
	≠	LPVC	-	A1.1	B1.2	
		HPVC	-	A1.1	B1.6	≥ 7,000
14	-	LPVC	-	A1.1	B1.2	
		HPVC	-	A1.1	B1.6	≥ 7,000
16	-	LPVC	-	A1.1	B1.2	
		HPVC	-	A1.1	B1.6	≥ 7,000
0	-	LPVC	-	A1.1	B1.2	
		HPVC	-	A1.1	B1.6	≥ 7,000

Annex 3 Identifiers for the target funnel

Identifier 1: Use category

Definition: The function categories / use categories represent various functional uses of substances.

Label: UC

Source: TGD (EC, 2003b)

Remarks: There are 55 use categories with a varying level of detail. For the examples in this report a subdivision was needed. Further development of the target funnel will require further diversification in function/use categories.

Identifier 2: Industrial category (production)

Definition: Industry in which the substance is produced (manufactured)

Label: IC

Source: TGD (EC, 2003b)

Remarks: In the TGD it is defined as the industry in which the substance is used. As all relevant life cycle stages have to be covered an extension for the life cycle stage has been added. In principle the industrial category for production should be different (IC 2 "Chemical industry: basic chemicals") from the industrial category for use of the substance. At present, however, for production in most cases the IC for production is the same as for (industrial) use.

Identifier 3: Production level

Definition: Annual production capacity at the site of a manufacturer, considering substances with an annual production volume < 1000 tonnes as an LPVC and ≥ 1000 tonnes as a HPVC

Label: PL

Source: TGD (EC, 2003b)

Remarks: In the A- and B-tables deviating limits for a HPVC are used depending on the industrial category and/or use category.

Identifier 4: Semi-finished preparation

Definition: Preparations that are formulated into chemical products

Label: SP

Source: Expert judgement, branch specific information, various ESDs etc.

Remarks: This identifier has been introduced because many substances undergo to formulation stages. In many industrial branches semi-finished reparations are characterised by the synonyms *additive packages* and *performance packages*.

Identifier 5: Industrial category (formulation 1)

Definition: Industry where the formulation of a semi-finished preparation takes place

Label: IC

Source: TGD (EC, 2003b)

Remark: See identifier 2

Identifier 6: Chemical products

Definition: Ready-for-use preparations for particular purposes like paints, inks, adhesives etc.

Label: CP

Source: Expert judgement, branch specific information, various ESDs etc.

Remarks: The list of chemical products in this report is a provisional one. Further development of this list should take into account presents product lists as for example TGD Volume II product use categories for consumer exposure assessment, US EPA list, and Nordic countries Products Register.

Identifier 7: Industrial category (formulation 2)

Definition: Industry where the formulation of a chemical products takes place

Label: IC

Source: TGD (EC, 2003b)

Remark: See identifier 2 and 5

Identifier 8: Type of use

Definition: The type of use describes the use of a substance as a processing aid in a certain process with the possibility that the substance ends up unintendedly in an article matrix and other uses where the substance goes into the article matrix or reacts during use or is part of a closed fluid system

Label: TU

Source: Expert judgement, branch specific information, various ESDs etc.

Identifier 9: Industrial category

Definition: Industry where the substance - as such or in a preparation - is used

Label: IC

Source: TGD (EC, 2003b)

Remark: See identifier 2, 5, and 7

Identifier 10: Process

Definition: Particular course of action intended to achieve a result

Label: PR

Source: http://www.wordreference.com/definition/process or expert judgement, branch specific information, various ESDs etc.

Remarks: Any process in industry may consist of a series of process steps in which a substance as such or in a formulation is used. A substance introduced in one of the process steps may pass to the next steps. In each of the following types there may be emission and the remainder may end up in the end product of the process. ***Example***: suppose that a process is defined as galvanic surface treatment of metal. Such a process comprises process steps such as (1) cleaning and degreasing, either by alkaline aqueous solutions or by vapour degreasing (2) acid dipping or mordant treatment and (3) electroplating.

Identifiers #: Any relevant identifier needed

Remarks: If the information provided by the identifiers 1to 10 is not sufficient one or more relevant identifiers have to be used. Such identifiers will have to be defined in the further development of the target funnel.

Annex 4 Idea for categorisation

For another structure of the industrial categories of the TGD in combination with the codes of NACE/NAICS and processes a survey was carried out for the overlap of the NACE codes and the Ics. NAICS codes are approximately the same as NACE codes and thus have not been dealt with separately. The results are too large to be presented completely in this report. They can be used, however, in restructuring the categorisation in order to define the complete matrix of emission scenarios that might be developed over the next years. As this will produce an enormous number of ESDs priority ranking in developing of ESDs should take place. In quite some cases ESDs for specific processes occurring in a multitude of industrial difficulties might be developed. Such ESDs then have to be developed only once with specific defaults for certain parameters (for example for the size of the process) for the various industrial branches. Furthermore, generic emission tables might be used for the least priorities. Probably the present A- and B-tables might be used with some alterations.

The results of the survey mentioned before can be used for the restructure of the ICs arranging them according to the life cycle stages. On the next page an impression is given how this might be done for the life cycle stages production, formulation and a small part of industrial use. The activities covered by the present ICs are presented in colours in order to show the overlap with the NACE codes of the various levels. As this is only a part of the complete survey it does not show the fact that various activities of a particular IC are split over various branches and main activities.

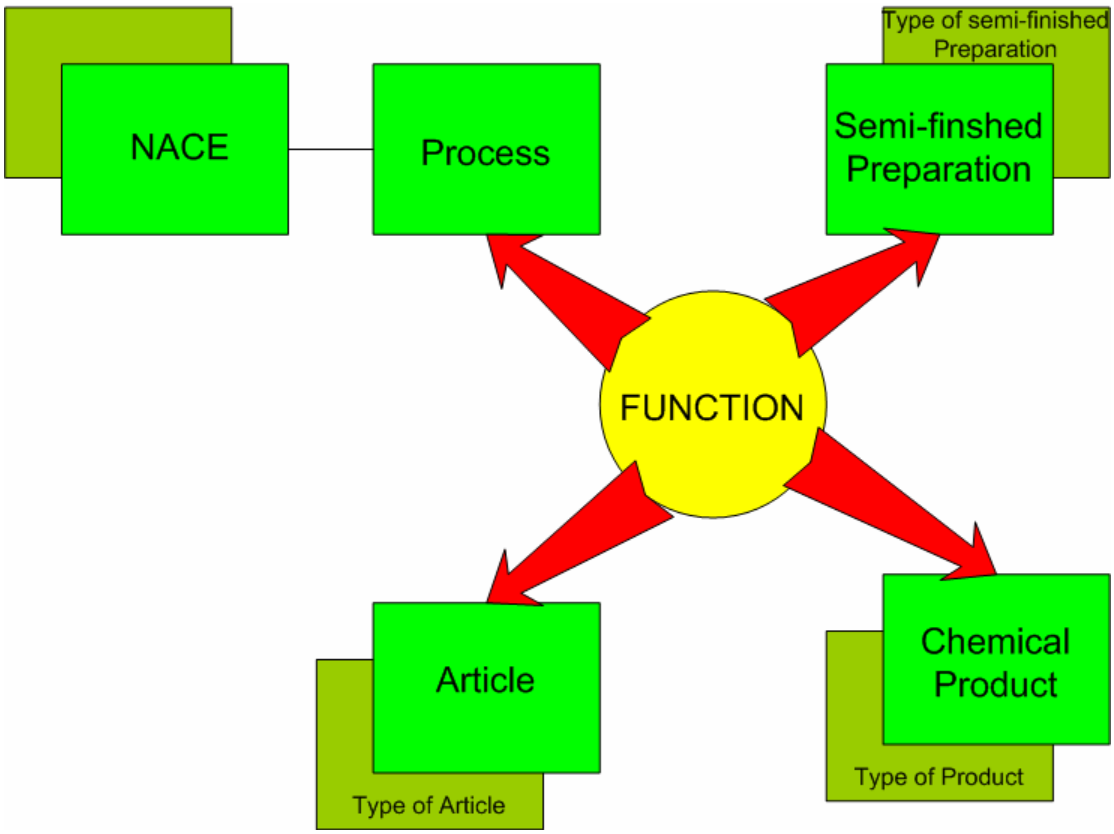
Life cycle stage	Branch	Main activity	Activity	IC	NACE codes
Production	Manufacturing	Manufacture of chemicals, chemical products and man-made fibres	Manufacture of dyes and pigments	2	2412
			Manufacture of other inorganic basic chemicals	2	2413
			Manufacture of other organic basic chemicals	2	2414
			Manufacture of basic pharmaceutical products	2	2441
			Manufacture of plastics in primary forms	11	2416
			Manufacture of synthetic rubber in primary forms	11	2417
Formulation			Manufacture of pharmaceutical preparations	2	2442
			manufacture of soap and detergents, cleaning and polishing preparations	2	2451
			Manufacture of perfumes and toilet preparations	2	2452
			Manufacture of glues and gelatines	2	2462
			manufacture of pesticides and other agro-chemical products	2	2420
			Manufacture of other chemical products n.e.c.	2	2466
			Manufacture of photographic chemical material	10	2464
			manufacture of paints, varnishes and similar coatings, printing ink and mastics	14	2430
Industrial use	Agriculture	Growing of crops	Growing of cereals and other crops n.e.c.	1	0111
			Growing of vegetables, horticultural specialities and nursery products	1	0112
			Growing of fruit, nuts, beverage and spice crops	1	0113
		Farming of animals	Farming of cattle, dairy farming	1	0121
			Farming of swine	1	0123
			Farming of poultry	1	0124
			Other farming of animals	1	0122, 0125
		Hunting	Hunting, trapping and game propagation, forestry and logging, operation of fish hatcheries and fish farms	1	0150, 0201, 0501, 0502
	Mining and quarrying	Energy producing materials	Mining and agglomeration of hard coal, lignite and peat	9	1010, 1020, 1030
			Extraction of crude petroleum and natural gas	9	1110
			Mining of uranium and thorium ores	9	1200
		Other materials	Mining of iron ores	8	1310
			Mining of non-ferrous metal ores, except uranium and thoriu	8	1320
			Quarrying of stone, limestone, gypsum, chalk and slate	0	1411-1413
			Operation of gravel and sand pits, and mining of clays and ka	0	1421, 1422
			Mining of chemical and fertilizer minerals	0	1430
			Production of salt	0	1440
			Other mining and quarrying n.e.c.	0	1450
	Manufacturing	Food and beverages manufacturing	Production and preserving of meat and poultry meat products	0	1511-1513
			Processing and preserving of fish and fish products	0	1520
			Processing and preserving of potatoes, fruit and vegetables; r	0	1531-1533

Annex 5 Life cycle stages for desired functions

Substances are used for all kinds of purposes and their function can be related to the following situations (see also the figure below):

- function during formulation process at manufacturing a semi-finished preparation or a chemical product;
- during use of the substance – as such or in a preparation – in a process;
- function of the substance during service life of a finished article.

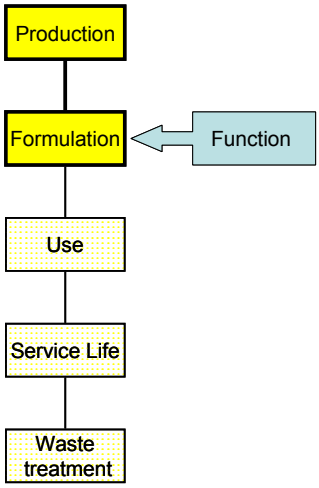
The various situations that can be considered are discussed below and examples are given.



1 Function during formulation

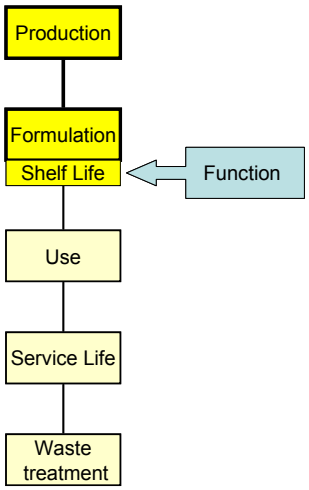
Substances which have a function during formulation are either released during formulation or incorporated into or onto a matrix. An ESD covering formulation and incorporating substances which have a specific function during formulation process should take into account the possibility that service life and waste treatment are important. Two examples are shown below.

Example 1: Milling aid in the manufacture of pigment paste



Substances with a function like this one usually will remain in the formulation (chemical product). So, the substance might be emitted during use of the chemical product completely. However, if the chemical product becomes part of the finished article the life cycle stages service life and waste treatment might be relevant. In case of this example the milling aid may become part of paint. After application of the paint (life cycle stage use) the milling aid becomes part of the coating matrix unless the vapour pressure of the substance is extremely high, which is not very likely. Furthermore, from the emission scenario it will appear which fraction will be emitted to air and hence which fraction will pass to the life cycle stage service life.

Example 2: Preservative to prolong the shelf life of aqueous adhesives

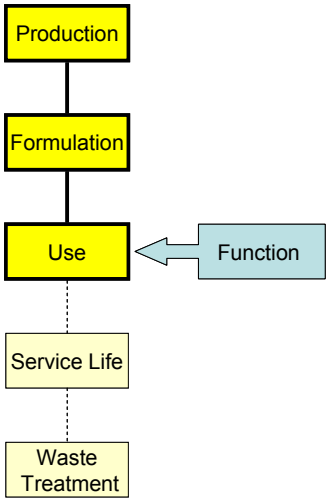


Substances with similar functions are an important component of a chemical product. By exerting their function they will be transformed into another substance. At application of the chemical product the remainder will become part of a matrix, in case of the example of the adhesive layer.

2 Function during use of formulation

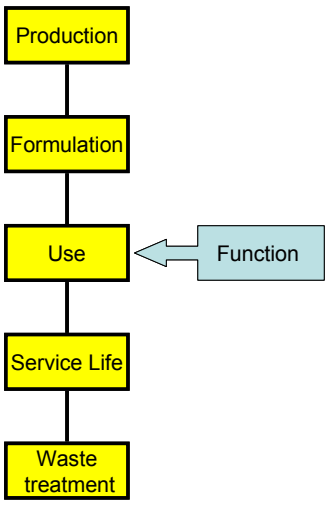
Substances that are formulated into a preparation (chemical product) and have a function during the use (life cycle stage of use for the substance) may or may not be incorporated in an end product. This is illustrated below with two examples.

Example 1: Release agent applied in mould release for rubber processing



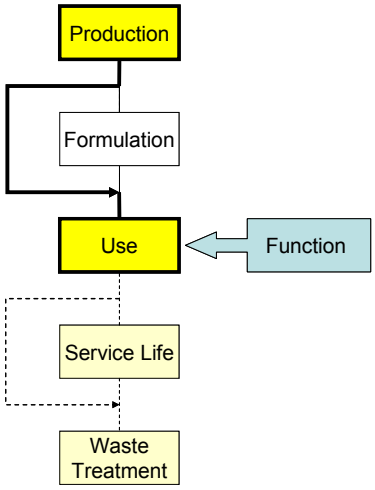
Despite the fact that the mould release should not remain on the rubber articles a certain fraction might remain on the surface. So, in principle this fraction could be considered is to have the life cycle stages service life and waste treatment. However, it is quite likely that in many cases the substance will be removed from the surface completely during article use in a short time and hence not enter the stage of waste treatment. This is shown in the figure by the broken line.

Example 2: Internal lubricant used in masterbatches for polymers processing industry



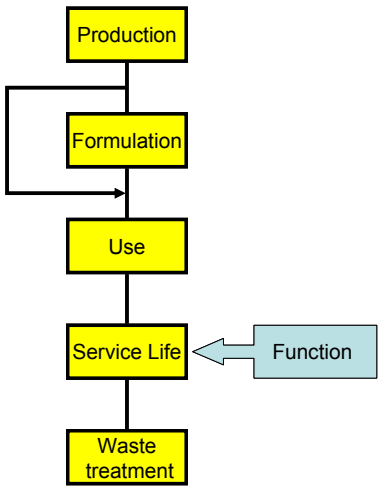
In a case like this the substance is included in a matrix deliberately. After its use - i.e. life cycle stage of use for the substance - the substance remains in a matrix of plastic articles and enter the stage of service life as such.

3 Function during use of substances (as such)



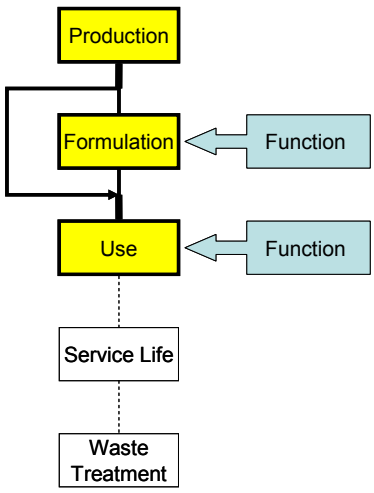
Substances used as such in a process as a processing aid may or may not be transferred to the matrix of finished articles. A catalyst used in a chemical reaction usually will not become part of a matrix. A possible exception is the uptake of a catalyst in a polymerisation reaction. After the reaction there is a possibility of the use/recovery/recycling (waste treatment) of the catalyst.

4 Function of the substance during service life of a finished article



The substance can be used as such or in the formulation for the manufacture of a article and exert its function during the service life of this article. Examples are substances like plasticizers used in PVC articles and pigments used in paint formulations for coating of substrates.

Function both at formulation and use



In principle a substance may have the same function in more than one stage of the life cycle. The only example at this moment is the use of a solvent in the formulation of a coating and at application of this coating for the dilution in order to obtain the right viscosity (for example to be able to use its in spray guns). During the drying or curing stage of the coating the solvent will be completely removed from the coating matrix. So, in the figure service life and waste treatment have been connected with broken lines and in white instead of yellow.